1-spar-Cl
Gas phase Energy: -1284.39082626681hartrees
Solvation Energy: -1284.40382464041hartrees
Zero Point Energy: 258.858 kcal/mol
Free Energy: -27.641 kcal/mol
final geometry:

| | angstroms | | |
|---|---|---|---|
| atom | x | y | z |
| Pd1 | -0.2033845924 | -0.0255909078 | 0.1373000963 |
| C2 | 0.0630221150 | 0.0828932431 | 3.6722449581 |
| C3 | 2.2616944253 | 0.0778745543 | 2.5801253095 |
| C4 | 1.8856852251 | -1.2248869836 | 1.8486004039 |
| N5 | 0.4147952970 | -1.4449580526 | 1.6787587426 |
| C6 | -0.3189373895 | -1.2426256108 | 2.9762331386 |
| C7 | -1.8232552624 | -1.4599404716 | 2.7722476701 |
| C8 | -2.1038609033 | -2.8905672780 | 2.2876892606 |
| C9 | -1.2759096191 | -3.2059677627 | 1.0340726870 |
| C10 | 0.2005680283 | -2.8567932791 | 1.2258160861 |
| C11 | 1.5712614187 | 0.0714809128 | 3.9526842990 |
| C12 | -0.2932534340 | 1.3906679790 | 2.9404700844 |
| N13 | 0.4716073875 | 1.6033759893 | 1.6862390241 |
| C14 | 1.9518406659 | 1.3937407089 | 1.8224996870 |
| C15 | 2.7010434998 | 2.5888869183 | 2.4629501534 |
| C16 | 0.8417800581 | 4.1244069325 | 1.7806905700 |
| C17 | 2.3611885119 | 3.9226372920 | 1.7854994876 |
| C18 | 0.1637218453 | 2.9360816745 | 1.0889589432 |
| H19 | -0.4935467975 | 0.0932544100 | 4.6181424744 |
| H20 | 3.3511656843 | 0.0414471396 | 2.7066644330 |
| H21 | 2.3364213241 | -1.2651288930 | 0.8530664958 |
| H22 | 2.2990048838 | -2.0625158280 | 2.4362274154 |
| H23 | 0.0338561816 | -2.0387149365 | 3.6586035012 |
| H24 | -2.3356976712 | -1.2698393157 | 3.7233823206 |
| H25 | -2.2024639543 | -0.7363009021 | 2.0407100846 |
| H26 | -1.8505544458 | -3.5987911839 | 3.0893972866 |
| H27 | -3.1712418050 | -3.0210792957 | 2.0790974221 |
| H28 | -1.3454146374 | -4.2706801243 | 0.7809743162 |
| H29 | -1.6631593413 | -2.6410315910 | 0.1803545479 |
| H30 | 0.7527278307 | -2.9865160484 | 0.2919114217 |
| H31 | 0.6463030527 | -3.5255586125 | 1.9823530372 |
| H32 | 1.8632776642 | 0.9351199015 | 4.5577470520 |
| H33 | 1.8552343778 | -0.8238884581 | 4.5192370683 |
| H34 | -0.1258788508 | 2.2140482492 | 3.6529935411 |
| H35 | -1.3539265857 | 1.4145067338 | 2.6725982345 |
| H36 | 2.3188282800 | 1.2969410270 | 0.7918820674 |

| | | | |
|---|---|---|---|
| H37 | 3.7776977591 | 2.3865650132 | 2.3997759171 |
| H38 | 2.4627217723 | 2.6660086244 | 3.5308715041 |
| H39 | 0.5690974325 | 5.0376576666 | 1.2389857267 |
| H40 | 0.4775116155 | 4.2526922343 | 2.8092778517 |
| H41 | 2.7288542887 | 3.9170090983 | 0.7500104197 |
| H42 | 2.8703202503 | 4.7472010960 | 2.2977441792 |
| H43 | -0.9244016334 | 3.0407530075 | 1.0736091234 |
| H44 | 0.4735501154 | 2.8977870410 | 0.0415667342 |
| H45 | -0.5579154718 | -1.1130752700 | -0.8657507625 |
| Cl46 | -0.8129167274 | 1.3624866126 | -1.6609628254 |

2-spar-Cl
Gas phase Energy: -1434.71019981287 hartrees
Solvation Energy: -1434.72217322666 hartrees
Zero Point Energy: 261.502 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | -0.5230771220 | -0.2484194665 | 0.1421080093 |
| C2 | 0.0658467236 | -0.0443251678 | 3.6216491376 |
| C3 | 2.1663124897 | -0.1932472022 | 2.3609382497 |
| C4 | 1.6698766663 | -1.4961593269 | 1.7061200229 |
| N5 | 0.1814307803 | -1.6495421411 | 1.6624718055 |
| C6 | -0.4305806169 | -1.3733050906 | 3.0085908542 |
| C7 | -1.9544512022 | -1.5313526669 | 2.9410559671 |
| C8 | -2.3332147533 | -2.9637703127 | 2.5345654946 |
| C9 | -1.6313584309 | -3.3565270166 | 1.2270570367 |
| C10 | -0.1309550702 | -3.0633659615 | 1.2760792638 |
| C11 | 1.5896294990 | -0.1209900605 | 3.7828033095 |
| C12 | -0.2867485025 | 1.2550983507 | 2.8721035480 |
| N13 | 0.3855706659 | 1.3888242973 | 1.5549384985 |
| C14 | 1.8601678203 | 1.1115335544 | 1.5843261540 |
| C15 | 2.7122055522 | 2.2878011030 | 2.1222522576 |
| C16 | 0.8813038206 | 3.8896488847 | 1.5237170546 |
| C17 | 2.3851507970 | 3.6124483616 | 1.4215431798 |
| C18 | 0.0957943750 | 2.7136991272 | 0.9322613656 |
| H19 | -0.4119664816 | 0.0254006048 | 4.6072829083 |
| H20 | 3.2594148101 | -0.2818546421 | 2.4011283239 |
| H21 | 2.0377955431 | -1.5873954644 | 0.6813737314 |
| H22 | 2.0894453235 | -2.3355878606 | 2.2865663857 |
| H23 | -0.0536831781 | -2.1616966882 | 3.6869808321 |
| H24 | -2.3743485027 | -1.2889612874 | 3.9251911624 |
| H25 | -2.3666806903 | -0.8161281594 | 2.2192276356 |
| H26 | -2.0396846083 | -3.6552928441 | 3.3371413204 |
| H27 | -3.4191591006 | -3.0547683043 | 2.4228425850 |

| | | | |
|---|---|---|---|
| H28 | -1.7635515943 | -4.4256203281 | 1.0218134637 |
| H29 | -2.0714522689 | -2.8066293203 | 0.3894245179 |
| H30 | 0.3302872769 | -3.2438248217 | 0.3019526619 |
| H31 | 0.3534813776 | -3.7285158842 | 2.0115945870 |
| H32 | 1.9695590471 | 0.7462735986 | 4.3311559927 |
| H33 | 1.8760316366 | -1.0105454694 | 4.3572673048 |
| H34 | -0.0244807270 | 2.0917540239 | 3.5390859195 |
| H35 | -1.3631210516 | 1.3225448040 | 2.6872188645 |
| H36 | 2.1425393591 | 0.9647297493 | 0.5341618488 |
| H37 | 3.7697543459 | 2.0290048260 | 1.9855865180 |
| H38 | 2.5608503265 | 2.4136476710 | 3.2012814565 |
| H39 | 0.6105810368 | 4.7957486086 | 0.9691131537 |
| H40 | 0.6041319840 | 4.0716069091 | 2.5711155963 |
| H41 | 2.6710758452 | 3.5518388840 | 0.3622211771 |
| H42 | 2.9709187972 | 4.4279037562 | 1.8613314344 |
| H43 | -0.9838323232 | 2.8725744399 | 0.9932775401 |
| H44 | 0.3224956857 | 2.6236035817 | -0.1331073678 |
| H45 | -1.0478825424 | -1.3436162263 | -0.7731849066 |
| O46 | 1.9801162082 | -0.7718692924 | -2.1716193628 |
| O47 | 2.9808174420 | -0.4030881539 | -1.5881825874 |
| Cl48 | -1.2947496441 | 1.1178455649 | -1.6114425492 |

3A-spar-Cl
Gas phase Energy: -1434.7285621014 hartrees
Solvation Energy: -1434.73888274838hartrees
Zero Point Energy: 263.465 kcal/mol
Free Energy: -30.272kcal/mol
final geometry:

| | angstroms | | |
|---|---|---|---|
| atom | x | y | z |
| Pd1 | -0.1236303052 | -0.0819611810 | 0.0617640885 |
| C2 | 0.0802992533 | 0.0496106215 | 3.6679476971 |
| C3 | 2.3110054689 | 0.0583950573 | 2.6447074133 |
| C4 | 1.9834541662 | -1.2708649089 | 1.9391039281 |
| N5 | 0.5310029415 | -1.5236194642 | 1.7415733026 |
| C6 | -0.2539960506 | -1.3017247856 | 2.9952687822 |
| C7 | -1.7476288308 | -1.5307627196 | 2.7302767841 |
| C8 | -2.0001953720 | -2.9642406342 | 2.2416293889 |
| C9 | -1.1243695228 | -3.2723257882 | 1.0204386001 |
| C10 | 0.3445422737 | -2.9262634804 | 1.2759187783 |
| C11 | 1.5784527872 | 0.0757305636 | 3.9949309508 |
| C12 | -0.2789306961 | 1.3315753339 | 2.8912665581 |
| N13 | 0.5177619814 | 1.5276494137 | 1.6538149491 |
| C14 | 1.9971184656 | 1.3444066591 | 1.8393222101 |
| C15 | 2.7026044441 | 2.5726303659 | 2.4676615537 |
| C16 | 0.8431507636 | 4.0571075257 | 1.6781566882 |

| | | | |
|---|---|---|---|
| C17 | 2.3642981924 | 3.8800680027 | 1.7400905991 |
| C18 | 0.2070974631 | 2.8357764828 | 1.0036225789 |
| H19 | -0.5057938437 | 0.0762568690 | 4.5955936179 |
| H20 | 3.3965027687 | 0.0522670593 | 2.8057165765 |
| H21 | 2.4607819370 | -1.3210553472 | 0.9551485561 |
| H22 | 2.4122609719 | -2.0833023005 | 2.5534822146 |
| H23 | 0.0674800919 | -2.0740161023 | 3.7218404271 |
| H24 | -2.3031414172 | -1.3348688429 | 3.6557555700 |
| H25 | -2.1002358941 | -0.8149007147 | 1.9764541435 |
| H26 | -1.7669538257 | -3.6681655774 | 3.0532300460 |
| H27 | -3.0587361326 | -3.1052492716 | 1.9972323679 |
| H28 | -1.1865925162 | -4.3338575025 | 0.7537478962 |
| H29 | -1.4779081708 | -2.7058308926 | 0.1528880597 |
| H30 | 0.9252290469 | -3.0514369992 | 0.3582409946 |
| H31 | 0.7635581202 | -3.6078288342 | 2.0383095576 |
| H32 | 1.8359661240 | 0.9596169541 | 4.5866573906 |
| H33 | 1.8605331410 | -0.7999992636 | 4.5921612288 |
| H34 | -0.1456899066 | 2.1767366448 | 3.5856155620 |
| H35 | -1.3322280973 | 1.3306139907 | 2.5946493063 |
| H36 | 2.3978250323 | 1.2263690115 | 0.8236329038 |
| H37 | 3.7839794118 | 2.3879602591 | 2.4470081183 |
| H38 | 2.4264979657 | 2.6756072853 | 3.5241145873 |
| H39 | 0.5741054186 | 4.9480835663 | 1.0990219368 |
| H40 | 0.4411622158 | 4.2095056381 | 2.6889984191 |
| H41 | 2.7674706723 | 3.8510059826 | 0.7181440980 |
| H42 | 2.8425699544 | 4.7276691922 | 2.2442441769 |
| H43 | -0.8811290283 | 2.9210898376 | 0.9480655946 |
| H44 | 0.5571646150 | 2.7712233323 | -0.0300429893 |
| O45 | -0.0455251898 | -1.6765876721 | -1.5210929906 |
| O46 | -0.2872599182 | -1.2913298936 | -2.7759306787 |
| H47 | -0.6021121295 | -0.3269454026 | -2.6702897194 |
| Cl48 | -1.0525567065 | 1.3598179627 | -1.8107474512 |

4-spar-Cl
Gas phase Energy: -1434.75082629915 hartrees
Solvation Energy: -1434.76569889242 hartrees
Zero Point Energy: 265.31 kcal/mol
Free Energy: -29.537 kcal/mol
final geometry:

| | angstroms | | |
|---|---|---|---|
| atom | x | y | z |
| Pd1 | 0.0101716536 | -0.0611242225 | 0.0396067276 |
| C2 | -0.0605287954 | 0.0560092979 | 3.5534579234 |
| C3 | 2.2176975702 | 0.0637518486 | 2.6379964887 |
| C4 | 1.9199282867 | -1.2640601627 | 1.9172194401 |
| N5 | 0.4704711071 | -1.5015168945 | 1.6361746606 |

| | | | |
|---|---|---|---|
| C6 | -0.3616742042 | -1.2924581652 | 2.8691317209 |
| C7 | -1.8425378605 | -1.5529241480 | 2.5727017292 |
| C8 | -2.0475940813 | -3.0114815295 | 2.1427947113 |
| C9 | -1.1507887336 | -3.3282053622 | 0.9409166996 |
| C10 | 0.3058387958 | -2.9205672996 | 1.1718183047 |
| C11 | 1.4200886512 | 0.0834131843 | 3.9507592518 |
| C12 | -0.3892128483 | 1.3259261347 | 2.7505767096 |
| N13 | 0.4719083310 | 1.5296065615 | 1.5497655013 |
| C14 | 1.9483047232 | 1.3547670005 | 1.8244157887 |
| C15 | 2.6139245497 | 2.5742549906 | 2.5096770405 |
| C16 | 0.7820839837 | 4.0656878186 | 1.6952044429 |
| C17 | 2.3002759791 | 3.9010342625 | 1.8099270667 |
| C18 | 0.1932814087 | 2.8723265832 | 0.9376200113 |
| H19 | -0.6905913936 | 0.0865547843 | 4.4513315090 |
| H20 | 3.2941695841 | 0.0530361461 | 2.8501810757 |
| H21 | 2.4524871570 | -1.3305083497 | 0.9639836657 |
| H22 | 2.2914721925 | -2.0799385320 | 2.5598952648 |
| H23 | -0.0391196206 | -2.0638785727 | 3.5928778770 |
| H24 | -2.4231902954 | -1.3266952654 | 3.4756646748 |
| H25 | -2.1877878740 | -0.8780763457 | 1.7796449847 |
| H26 | -1.8073966730 | -3.6723020963 | 2.9884757223 |
| H27 | -3.0976909760 | -3.1925588856 | 1.8889919209 |
| H28 | -1.1614212164 | -4.4029652968 | 0.7223841929 |
| H29 | -1.5205822913 | -2.8164491236 | 0.0513379628 |
| H30 | 0.8647781142 | -3.0266827103 | 0.2409484169 |
| H31 | 0.7648829882 | -3.5649719550 | 1.9404858541 |
| H32 | 1.6494757538 | 0.9659620626 | 4.5551114698 |
| H33 | 1.6716902134 | -0.7918735182 | 4.5615200651 |
| H34 | -0.2933548163 | 2.1805479940 | 3.4355419475 |
| H35 | -1.4240245275 | 1.3137445573 | 2.3967174661 |
| H36 | 2.4041138286 | 1.2500147103 | 0.8317404815 |
| H37 | 3.6953421179 | 2.3906898660 | 2.5262871560 |
| H38 | 2.2977429900 | 2.6482384884 | 3.5567562361 |
| H39 | 0.5253868204 | 4.9734359160 | 1.1370316663 |
| H40 | 0.3376030346 | 4.1790911336 | 2.6931397882 |
| H41 | 2.7433270102 | 3.9082043922 | 0.8047488760 |
| H42 | 2.7515931210 | 4.7332106722 | 2.3619835895 |
| H43 | -0.8901263004 | 2.9512320701 | 0.8211621583 |
| H44 | 0.6037428160 | 2.8509774465 | -0.0724904760 |
| O45 | -0.1237395915 | -1.5296472009 | -1.2701614745 |
| O46 | -1.4272413252 | -1.5482395370 | -1.8561979435 |
| H47 | -1.3818746550 | -0.7518298731 | -2.4208430922 |
| Cl48 | -0.4478882148 | 1.4040508012 | -1.8302089340 |

TS1-spar-Cl
Gas phase Energy: -1434.68770510733 hartrees

Solvation Energy: -1434.70042028364 hartrees
Zero Point Energy: 259.299 kcal/mol
Free Energy: -31.732 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1563.55 $cm^{-1}$)
final geometry:

| | angstroms | | |
|---|---|---|---|
| atom | x | y | z |
| Pd1 | -0.1645640110 | -0.1112261236 | 0.0796542640 |
| C2 | 0.0491733220 | 0.0463459570 | 3.6184063773 |
| C3 | 2.2686123753 | 0.0426455956 | 2.5670863409 |
| C4 | 1.9150135179 | -1.2694770244 | 1.8413086967 |
| N5 | 0.4499454582 | -1.5035142183 | 1.6515891287 |
| C6 | -0.3112961413 | -1.2889568365 | 2.9303756498 |
| C7 | -1.8104415090 | -1.5170678277 | 2.6991956885 |
| C8 | -2.0726322581 | -2.9552412100 | 2.2283012635 |
| C9 | -1.2239666909 | -3.2723388683 | 0.9911952984 |
| C10 | 0.2498516463 | -2.9174813051 | 1.2027994516 |
| C11 | 1.5521433923 | 0.0473594979 | 3.9261217739 |
| C12 | -0.3026007561 | 1.3437097943 | 2.8660733324 |
| N13 | 0.4859751154 | 1.5458573731 | 1.6267602639 |
| C14 | 1.9632257834 | 1.3468217001 | 1.7890377479 |
| C15 | 2.6853075172 | 2.5597801809 | 2.4267554187 |
| C16 | 0.8303724869 | 4.0665028962 | 1.6633307544 |
| C17 | 2.3506214196 | 3.8764127653 | 1.7134693769 |
| C18 | 0.1777483808 | 2.8564343303 | 0.9844642014 |
| H19 | -0.5247805379 | 0.0638698325 | 4.5535767977 |
| H20 | 3.3556517350 | 0.0157439142 | 2.7143336736 |
| H21 | 2.3813427812 | -1.3143262283 | 0.8526452190 |
| H22 | 2.3280804293 | -2.0991264051 | 2.4399659204 |
| H23 | 0.0306981300 | -2.0751303929 | 3.6291913740 |
| H24 | -2.3436374204 | -1.3154769258 | 3.6362461580 |
| H25 | -2.1802582400 | -0.8060635516 | 1.9497066945 |
| H26 | -1.8233763865 | -3.6523433606 | 3.0406988562 |
| H27 | -3.1355350834 | -3.0979656753 | 2.0053949532 |
| H28 | -1.2841197320 | -4.3366709292 | 0.7361089267 |
| H29 | -1.6093808013 | -2.7186627804 | 0.1301282380 |
| H30 | 0.8104183069 | -3.0569801676 | 0.2750558551 |
| H31 | 0.6868404647 | -3.5819120364 | 1.9680097500 |
| H32 | 1.8281746224 | 0.9190766127 | 4.5270594419 |
| H33 | 1.8301472754 | -0.8403161379 | 4.5072616893 |
| H34 | -0.1530799663 | 2.1770904068 | 3.5711236315 |
| H35 | -1.3580975665 | 1.3590265582 | 2.5778059459 |
| H36 | 2.3498078079 | 1.2419780024 | 0.7664402643 |
| H37 | 3.7648748483 | 2.3664530446 | 2.3947867065 |
| H38 | 2.4179561794 | 2.6539372112 | 3.4863010754 |
| H39 | 0.5659083229 | 4.9635144696 | 1.0913961243 |

| | | | |
|---|---|---|---|
| H40 | 0.4366438576 | 4.2165375896 | 2.6778445584 |
| H41 | 2.7464706415 | 3.8530876239 | 0.6886612713 |
| H42 | 2.8386015822 | 4.7158155449 | 2.2219313471 |
| H43 | -0.9102954321 | 2.9503743942 | 0.9402374258 |
| H44 | 0.5152990537 | 2.7930583834 | -0.0530237663 |
| H45 | -0.3566734431 | -1.2802620381 | -1.1018567523 |
| O46 | -0.5048880263 | -2.1496946216 | -2.0887462914 |
| O47 | 0.3031563916 | -3.1160972666 | -2.0222480983 |
| Cl48 | -0.8309783776 | 1.2173200785 | -1.7516832062 |

5,6-spar-Cl
Gas phase Energy: -1744.02030989879 hartrees
Solvation Energy: -1744.03706954214 hartrees
Zero Point Energy: 255.248 kcal/mol
Free Energy: -28.742 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.0079508626 | 0.0123718936 | 0.0028620697 |
| C2 | -0.0352869628 | -0.0247144084 | 3.5267202676 |
| C3 | 2.2344537673 | -0.0453668305 | 2.5870966585 |
| C4 | 1.9028026958 | -1.3305772094 | 1.8103142708 |
| N5 | 0.4465625473 | -1.5118526664 | 1.5288263587 |
| C6 | -0.3871218450 | -1.3171546398 | 2.7684980206 |
| C7 | -1.8760523021 | -1.4929485513 | 2.4458564315 |
| C8 | -2.1495988233 | -2.9213478631 | 1.9572742252 |
| C9 | -1.2365173386 | -3.2508513966 | 0.7712681542 |
| C10 | 0.2306564492 | -2.9227104666 | 1.0528717965 |
| C11 | 1.4494217040 | -0.0659819146 | 3.9083269284 |
| C12 | -0.3355955678 | 1.2915730810 | 2.7968313946 |
| N13 | 0.5076796896 | 1.5174100436 | 1.5878889084 |
| C14 | 1.9869846216 | 1.2850308440 | 1.8328629686 |
| C15 | 2.6978145152 | 2.4492817984 | 2.5694405762 |
| C16 | 0.9026763440 | 4.0325227446 | 1.8738197546 |
| C17 | 2.4161393294 | 3.8222435977 | 1.9531936910 |
| C18 | 0.2702138086 | 2.9034999094 | 1.0556415217 |
| H19 | -0.6563288275 | -0.0264287618 | 4.4312581406 |
| H20 | 3.3121019899 | -0.0868282451 | 2.7879469361 |
| H21 | 2.4244051858 | -1.3683269287 | 0.8497279525 |
| H22 | 2.2542335583 | -2.1837769084 | 2.4133971776 |
| H23 | -0.1057774962 | -2.1382168008 | 3.4519791468 |
| H24 | -2.4564318546 | -1.2736148015 | 3.3505628100 |
| H25 | -2.1786180199 | -0.7707950640 | 1.6773953285 |
| H26 | -1.9711970557 | -3.6238107789 | 2.7840664034 |
| H27 | -3.2005388103 | -3.0328701749 | 1.6696971006 |
| H28 | -1.2955579550 | -4.3159388895 | 0.5177573012 |

| | | | |
|---|---|---|---|
| H29 | -1.5514454745 | -2.6974762856 | -0.1165146939 |
| H30 | 0.8251594179 | -3.0592260947 | 0.1497018752 |
| H31 | 0.6228690655 | -3.5856600718 | 1.8416001806 |
| H32 | 1.7127253064 | 0.7762351733 | 4.5547397116 |
| H33 | 1.6775398484 | -0.9791450542 | 4.4705849295 |
| H34 | -0.1869219115 | 2.1097041815 | 3.5151043790 |
| H35 | -1.3771704124 | 1.3371619840 | 2.4678968517 |
| H36 | 2.4251514558 | 1.2151360463 | 0.8300458092 |
| H37 | 3.7723829747 | 2.2301098459 | 2.5554430483 |
| H38 | 2.4023580863 | 2.4734841262 | 3.6247085775 |
| H39 | 0.6605061860 | 4.9757581359 | 1.3708544270 |
| H40 | 0.4756774173 | 4.1020403834 | 2.8832284201 |
| H41 | 2.8450864807 | 3.8772525711 | 0.9435150335 |
| H42 | 2.8988796788 | 4.6065462585 | 2.5469929863 |
| H43 | -0.8094637974 | 3.0244304042 | 0.9514149009 |
| H44 | 0.6736346499 | 2.9278718757 | 0.0435633495 |
| Cl45 | 0.0727710520 | -1.5135683666 | -1.7918788337 |
| Cl46 | -0.6831199723 | 1.5969909914 | -1.5931149335 |

1-bipyr-Cl
Gas phase Energy: -1082.99831472470 hartrees
Solvation Energy: -1083.01498336014hartrees
Zero Point Energy: 106.467 kcal/mol
Free Energy: -25.338 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | .1025425149 | 1.3815374069 | -2.0379855191 |
| N2 | .4208234633 | 1.9030842361 | .0875547677 |
| N3 | -1.6666918681 | 2.3755137588 | -1.5315747824 |
| C4 | 1.5105216071 | 1.6199046935 | .8085554162 |
| C5 | 1.6262253184 | 1.9906228579 | 2.1482845101 |
| C6 | .5675092028 | 2.6763035172 | 2.7413983271 |
| C7 | -.5665126217 | 2.9693247721 | 1.9862820648 |
| C8 | -.6146606441 | 2.5665282985 | .6460894741 |
| C9 | -1.7715329526 | 2.8256587270 | -.2503826075 |
| C10 | -2.9237508170 | 3.4970584715 | .1741097545 |
| C11 | -3.9720868922 | 3.7088869376 | -.7159381729 |
| C12 | -3.8508916757 | 3.2436048008 | -2.0237344898 |
| C13 | -2.6825976612 | 2.5828627527 | -2.3891493966 |
| H14 | 2.2909202785 | 1.0838231289 | .2748281446 |
| H15 | 2.5237934822 | 1.7458067250 | 2.7052759007 |
| H16 | .6194636914 | 2.9822953295 | 3.7816960817 |
| H17 | -1.3927487223 | 3.5021702309 | 2.4409374386 |
| H18 | -3.0034618953 | 3.8527360350 | 1.1937251779 |

| | | | |
|---|---|---|---|
| H19 | -4.8673821453 | 4.2289494538 | -.3909400375 |
| H20 | -4.6398777614 | 3.3846279434 | -2.7536751597 |
| H21 | -2.5333311553 | 2.2003078399 | -3.3904824974 |
| Cl22 | 2.1304366141 | .2929203517 | -2.4520730858 |
| H23 | -.2448674481 | 1.0857018393 | -3.4948986842 |

2- bipyr-Cl
Gas phase Energy: -1233.31673859978 hartrees
Solvation Energy: -1233.3326862228 hartrees
Zero Point Energy: 109.071 kcal/mol
Free Energy: -30.907 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | .4532763414 | .1261927740 | -.1663349621 |
| N2 | .2108933327 | .1191078968 | 1.9131944023 |
| N3 | 2.5351502695 | .0158976657 | .5721378423 |
| C4 | -.9831802128 | .1729001895 | 2.5308812639 |
| C5 | -1.1121458182 | .1694627714 | 3.9162533997 |
| C6 | .0424499100 | .1075600552 | 4.6936009026 |
| C7 | 1.2791457189 | .0512692767 | 4.0584520328 |
| C8 | 1.3475123787 | .0578692887 | 2.6607848905 |
| C9 | 2.6342076648 | .0002195017 | 1.9190169747 |
| C10 | 3.8859719687 | -.0661781871 | 2.5429405932 |
| C11 | 5.0342107706 | -.1161793853 | 1.7548965053 |
| C12 | 4.9126569908 | -.0991608237 | .3664856971 |
| C13 | 3.6342727241 | -.0320037938 | -.1875398809 |
| H14 | -1.8466173593 | .2190552077 | 1.8800033496 |
| H15 | -2.0983020417 | .2146620721 | 4.3642892673 |
| H16 | -.0152746171 | .1029816408 | 5.7773017720 |
| H17 | 2.1854942960 | .0027201585 | 4.6489326317 |
| H18 | 3.9736205847 | -.0790178509 | 3.6224917484 |
| H19 | 6.0115669056 | -.1678092464 | 2.2246076063 |
| H20 | 5.7838361554 | -.1367677703 | -.2780240279 |
| H21 | 3.4557143943 | -.0145847660 | -1.2595391835 |
| H22 | -1.0227870868 | .2030517346 | -.5395920901 |
| O23 | -3.8165083521 | -.3919112124 | -.5836305104 |
| O24 | -4.0858429314 | .0053846379 | .5318611906 |
| Cl25 | .8736460718 | .1280135236 | -2.4663301091 |

3A- bipyr-Cl
Gas phase Energy: -1233.33457321476 hartrees
Solvation Energy: -1233.34856323605 hartrees
Zero Point Energy: 111.121 kcal/mol
Free Energy: -28.556 kcal/mol
final geometry:

| | angstroms | | |
|---|---|---|---|
| atom | x | y | z |
| Pd1 | -0.0699106870 | 1.1320165194 | -1.9036577560 |
| N2 | 0.1735944821 | 1.8845970501 | 0.1997021228 |
| N3 | -1.7208255889 | 2.5848708207 | -1.5819998627 |
| C4 | 1.1385064268 | 1.4806312780 | 1.0368057758 |
| C5 | 1.2473340542 | 1.9539716125 | 2.3427867280 |
| C6 | 0.3089966597 | 2.8839897053 | 2.7872679259 |
| C7 | -0.6944766249 | 3.3044598243 | 1.9183086147 |
| C8 | -0.7424436601 | 2.7873989978 | 0.6170366737 |
| C9 | -1.7836053727 | 3.1846144295 | -0.3735652305 |
| C10 | -2.7843121888 | 4.1243012501 | -0.0967857427 |
| C11 | -3.7199855772 | 4.4344645640 | -1.0813420572 |
| C12 | -3.6404899636 | 3.8043129442 | -2.3219213754 |
| C13 | -2.6176459148 | 2.8807315784 | -2.5310297544 |
| H14 | 1.8379070273 | 0.7544831953 | 0.6333723520 |
| H15 | 2.0448839471 | 1.5996698326 | 2.9864802505 |
| H16 | 0.3542988640 | 3.2785318046 | 3.7975612079 |
| H17 | -1.4294634672 | 4.0246391637 | 2.2561629782 |
| H18 | -2.8388858321 | 4.6121395637 | 0.8687436345 |
| H19 | -4.5004246714 | 5.1610326336 | -0.8780800100 |
| H20 | -4.3496112905 | 4.0182363161 | -3.1137497618 |
| H21 | -2.4910237227 | 2.3516221507 | -3.4713263006 |
| H22 | 1.1203837409 | -0.6023448804 | -3.6408803963 |
| O23 | 1.6451683295 | -0.2375980450 | -1.8956231821 |
| O24 | 1.8609066496 | -0.9208598090 | -3.0216613161 |
| Cl25 | -0.4847255807 | 0.3944895908 | -4.2813081459 |

4- bipyr-Cl
Gas phase Energy: -1233.36137111896 hartrees
Solvation Energy: -1233.38050898649 hartrees
Zero Point Energy: 112.709 kcal/mol
Free Energy: -27.099 kcal/mol
final geometry:

| | angstroms | | |
|---|---|---|---|
| atom | x | y | z |
| Pd1 | 0.0077203179 | 1.2677662484 | -1.9578868403 |
| N2 | 0.2233265962 | 1.8289861424 | 0.0268913324 |
| N3 | -1.6646850030 | 2.5430629911 | -1.6948888822 |
| C4 | 1.2175519159 | 1.3794611890 | 0.8037307280 |
| C5 | 1.3236747601 | 1.7627310439 | 2.1386695304 |
| C6 | 0.3664576462 | 2.6306571908 | 2.6632027808 |
| C7 | -0.6648898810 | 3.0907119546 | 1.8458785851 |
| C8 | -0.7199440592 | 2.6727323473 | 0.5132783613 |
| C9 | -1.7683244709 | 3.0814718500 | -0.4523894098 |
| C10 | -2.8127146788 | 3.9568815480 | -0.1427161075 |

| | | | |
|---|---|---|---|
| C11 | -3.7526099878 | 4.2714261232 | -1.1224742335 |
| C12 | -3.6318286002 | 3.7060526925 | -2.3903158961 |
| C13 | -2.5668363375 | 2.8415139498 | -2.6395970446 |
| H14 | 1.9074246375 | 0.7054423305 | 0.3009344602 |
| H15 | 2.1382353864 | 1.3842885218 | 2.7458570972 |
| H16 | 0.4178589964 | 2.9477542433 | 3.6999002260 |
| H17 | -1.4149187618 | 3.7629157993 | 2.2447751752 |
| H18 | -2.8941283037 | 4.3896578208 | 0.8471036242 |
| H19 | -4.5677102811 | 4.9508557594 | -0.8942590417 |
| H20 | -4.3429895890 | 3.9261288712 | -3.1785106640 |
| H21 | -2.4030030530 | 2.3638325597 | -3.6009472779 |
| H22 | 1.2401991411 | -1.1504770395 | -3.1225632427 |
| O23 | 1.6630680669 | 0.2096832512 | -1.9010052765 |
| O24 | 1.3539864669 | -1.1633155511 | -2.1547357834 |
| Cl25 | -0.3845572112 | 0.7164657390 | -4.2445088309 |

TS1- bipyr-Cl
Gas phase Energy: -1233.29530813908 hartrees
Solvation Energy: -1233.31008381439 hartrees
Zero Point Energy: 106.873 kcal/mol
Free Energy: -29.356 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1621.30 $cm^{-1}$)
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | .3106450294 | .0733792027 | -.1276718595 |
| N2 | .1399376547 | .0788349054 | 1.9780922645 |
| N3 | 2.4312735518 | .0464698348 | .5720624131 |
| C4 | -1.0375380090 | .1028240286 | 2.6261449813 |
| C5 | -1.1263660406 | .1167501278 | 4.0158430074 |
| C6 | .0509669168 | .1060302219 | 4.7598559624 |
| C7 | 1.2711061524 | .0798702968 | 4.0905187158 |
| C8 | 1.2987069663 | .0651070918 | 2.6918367086 |
| C9 | 2.5654253695 | .0344485031 | 1.9145403759 |
| C10 | 3.8353552341 | -.0066088682 | 2.5032915018 |
| C11 | 4.9620466240 | -.0336497243 | 1.6837618649 |
| C12 | 4.8026316571 | -.0197159826 | .2989678615 |
| C13 | 3.5084972586 | .0200729446 | -.2193595328 |
| H14 | -1.9247340127 | .1092600770 | 1.9993427963 |
| H15 | -2.1002897008 | .1360312195 | 4.4916284880 |
| H16 | .0245052627 | .1178642099 | 5.8448073756 |
| H17 | 2.1947477584 | .0726094122 | 4.6556634788 |
| H18 | 3.9529840565 | -.0199015218 | 3.5800322427 |
| H19 | 5.9525909706 | -.0660218467 | 2.1263575253 |
| H20 | 5.6563821800 | -.0403124093 | -.3693071664 |
| H21 | 3.3019867199 | .0310961551 | -1.2860742554 |

| | | | |
|---|---|---|---|
| H22 | -1.3309483829 | .0726577306 | -.5035954209 |
| O23 | -2.6208400163 | .0660870263 | -.7654113977 |
| O24 | -3.3218271930 | .0646471593 | .2839965298 |
| Cl25 | .6118801288 | .0625400911 | -2.4485223903 |

1-bipyr-$CH_3$
Gas phase Energy: -662.66064953707 hartrees
Solvation Energy: -662.67161037637 hartrees
Zero Point Energy: 127.637 kcal/mol
Free Energy: -26.440 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.0078274022 | 1.1692799951 | -2.0318428305 |
| N2 | 0.1935151876 | 1.8094243986 | 0.0669334619 |
| N3 | -1.6803451465 | 2.6214889787 | -1.6816794022 |
| C4 | 1.1619625157 | 1.3772272846 | 0.8872278371 |
| C5 | 1.2872095903 | 1.8103386917 | 2.2047440604 |
| C6 | 0.3652465843 | 2.7358434524 | 2.6883622278 |
| C7 | -0.6419245014 | 3.1874558374 | 1.8419117911 |
| C8 | -0.7095982401 | 2.7054604606 | 0.5279317693 |
| C9 | -1.7597187058 | 3.1373047063 | -0.4336682230 |
| C10 | -2.7854620770 | 4.0256903512 | -0.0842017788 |
| C11 | -3.7353454272 | 4.3852037717 | -1.0347248584 |
| C12 | -3.6429498444 | 3.8493137221 | -2.3170413636 |
| C13 | -2.5971922825 | 2.9705273200 | -2.5915171765 |
| H14 | 1.8508092898 | 0.6602716324 | 0.4550099576 |
| H15 | 2.0890904812 | 1.4295322056 | 2.8282254688 |
| H16 | 0.4269023469 | 3.1031121665 | 3.7084328531 |
| H17 | -1.3628930604 | 3.9099832771 | 2.2050879382 |
| H18 | -2.8495442447 | 4.4322692475 | 0.9179372825 |
| H19 | -4.5349030021 | 5.0724005748 | -0.7741335644 |
| H20 | -4.3613906849 | 4.1008330931 | -3.0899353455 |
| H21 | -2.4784064461 | 2.5224054960 | -3.5729654831 |
| H22 | 1.1857044263 | 0.1750739100 | -2.1767983420 |
| C23 | -0.2232694758 | 0.6374914211 | -3.9914954545 |
| H24 | -1.0542041956 | 1.2259002166 | -4.4085078081 |
| H25 | 0.6768938439 | 0.8436909155 | -4.5775698265 |
| H26 | -0.4636843735 | -0.4258544602 | -4.0868176282 |

2- bipyr- $CH_3$
Gas phase Energy: -812.97899435790 hartrees
Solvation Energy: -812.98926027226 hartrees
Zero Point Energy: 130.185 kcal/mol
Free Energy: -30.647 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.4629886526 | 0.0695558773 | -0.2323059003 |
| N2 | 0.2473751394 | 0.0780947809 | 1.9614500917 |
| N3 | 2.5607880844 | 0.0318094604 | 0.5907707939 |
| C4 | -0.9400689218 | 0.1133351125 | 2.5852472914 |
| C5 | -1.0632143713 | 0.1520680499 | 3.9721624666 |
| C6 | 0.0992645451 | 0.1561119482 | 4.7410077527 |
| C7 | 1.3331593458 | 0.1188082381 | 4.0984279428 |
| C8 | 1.3829744854 | 0.0778347891 | 2.6987689811 |
| C9 | 2.6623181459 | 0.0331003481 | 1.9399060926 |
| C10 | 3.9152623554 | -0.0087778923 | 2.5673145325 |
| C11 | 5.0703978428 | -0.0501439570 | 1.7915257829 |
| C12 | 4.9526716509 | -0.0503774935 | 0.4027844063 |
| C13 | 3.6742984120 | -0.0093696554 | -0.1502463194 |
| H14 | -1.8084980960 | 0.1106312886 | 1.9364768343 |
| H15 | -2.0464268937 | 0.1796375646 | 4.4289363836 |
| H16 | 0.0496675733 | 0.1884731308 | 5.8249072619 |
| H17 | 2.2433460143 | 0.1245100193 | 4.6853037264 |
| H18 | 3.9953182127 | -0.0122459544 | 3.6473984381 |
| H19 | 6.0456960057 | -0.0827332037 | 2.2673051743 |
| H20 | 5.8246401820 | -0.0825388947 | -0.2413419925 |
| H21 | 3.5229026500 | -0.0090993523 | -1.2250539087 |
| H22 | -1.0078286700 | 0.0873509347 | -0.7140528524 |
| O23 | -3.8633326426 | -0.0191779614 | -0.6702457887 |
| O24 | -4.0985472643 | 0.0398561676 | 0.5199063323 |
| C25 | 0.7496237387 | 0.0826345976 | -2.2559999977 |
| H26 | 1.8292432098 | 0.1796455819 | -2.4463785887 |
| H27 | 0.3959092032 | -0.8493210328 | -2.7069182717 |
| H28 | 0.2361669586 | 0.9180410763 | -2.7383545318 |

3A- bipyr- $CH_3$
Gas phase Energy: -812.96300567677 hartrees
Solvation Energy: -812.97232741706 hartrees
Zero Point Energy: 132.058 kcal/mol
Free Energy: -29.930 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.0146635658 | 1.2358572495 | -2.0287456931 |
| N2 | 0.2844457765 | 2.0193830570 | 0.0949245589 |
| N3 | -1.9100956036 | 2.3342768280 | -1.4832107582 |
| C4 | 1.2735303403 | 1.6445961202 | 0.9196941637 |
| C5 | 1.3096422021 | 2.0005894911 | 2.2642788175 |
| C6 | 0.2556390418 | 2.7599118808 | 2.7794373337 |
| C7 | -0.7851609436 | 3.1293311434 | 1.9362645819 |

| | | | |
|---|---|---|---|
| C8 | -0.7448601636 | 2.7510950569 | 0.5852787639 |
| C9 | -1.8080513172 | 3.1129872039 | -0.3736377366 |
| C10 | -2.6676611710 | 4.2033328420 | -0.1691402762 |
| C11 | -3.6732726799 | 4.4657391191 | -1.0905680506 |
| C12 | -3.7921281772 | 3.6384495854 | -2.2135423164 |
| C13 | -2.8809336376 | 2.6027808284 | -2.3736951426 |
| H14 | 2.0526476568 | 1.0367459737 | 0.4693756991 |
| H15 | 2.1390729362 | 1.6868324300 | 2.8888595102 |
| H16 | 0.2372753163 | 3.0448126855 | 3.8272704940 |
| H17 | -1.6346485146 | 3.6805767548 | 2.3239652036 |
| H18 | -2.5351457741 | 4.8468846747 | 0.6938336993 |
| H19 | -4.3466290990 | 5.3049305200 | -0.9443243785 |
| H20 | -4.5716211140 | 3.7960621115 | -2.9515433116 |
| H21 | -2.9115946473 | 1.9510106209 | -3.2412956952 |
| H22 | 0.9715974238 | -1.0000684787 | -3.2727575447 |
| O23 | 1.5018836914 | -0.2126574532 | -1.6873461271 |
| O24 | 1.4867532945 | -1.3185781865 | -2.5025118175 |
| C25 | -0.3374035694 | 0.8164890696 | -4.0773356926 |
| H26 | -0.6071313816 | 1.7532286930 | -4.5792470404 |
| H27 | 0.5469879537 | 0.4253047266 | -4.6016270253 |
| H28 | -1.1668149915 | 0.1077057739 | -4.1994722329 |

3B- bipyr- $CH_3$
Gas phase Energy: -812.96105504788 hartrees
Solvation Energy: -812.96975033414 hartrees
Zero Point Energy: 131.194 kcal/mol
Free Energy: -29.090 kcal/mol
final geometry:

| | angstroms | | |
|---|---|---|---|
| atom | x | y | z |
| Pd1 | 0.3046046712 | 0.0333790177 | -0.2055788594 |
| N2 | 0.1650351295 | 0.0781221095 | 2.0140477325 |
| N3 | 2.4789048834 | 0.0255896944 | 0.6198944537 |
| C4 | -1.0158498648 | 0.0989502955 | 2.6540350328 |
| C5 | -1.1177678269 | 0.1041201055 | 4.0439892866 |
| C6 | 0.0546889124 | 0.0867122201 | 4.7959207511 |
| C7 | 1.2798295754 | 0.0666184774 | 4.1352358315 |
| C8 | 1.3114561429 | 0.0635404452 | 2.7345133724 |
| C9 | 2.5877608280 | 0.0437187419 | 1.9648126989 |
| C10 | 3.8478362915 | 0.0444100992 | 2.5809571753 |
| C11 | 4.9952734246 | 0.0250367186 | 1.7926243514 |
| C12 | 4.8664855019 | 0.0060134864 | 0.4048016447 |
| C13 | 3.5816311399 | 0.0074991052 | -0.1354126450 |
| H14 | -1.8968464718 | 0.1122623761 | 2.0168169360 |
| H15 | -2.0947418666 | 0.1207864737 | 4.5143641942 |
| H16 | 0.0209455935 | 0.0885938818 | 5.8810070154 |

| | | | |
|---|---|---|---|
| H17 | 2.1975848332 | 0.0519495414 | 4.7099930742 |
| H18 | 3.9409095427 | 0.0609541260 | 3.6599236240 |
| H19 | 5.9755858146 | 0.0252552493 | 2.2591394555 |
| H20 | 5.7339307488 | -0.0093717673 | -0.2461372026 |
| H21 | 3.4158423802 | -0.0065824028 | -1.2085849970 |
| H22 | -1.7823155330 | 0.1376389333 | -0.7519267939 |
| O23 | -2.7882590512 | 0.1804953357 | -0.9186255344 |
| O24 | -3.3738767597 | 0.1781420979 | 0.2673031404 |
| C25 | 0.4731750610 | -0.0249468318 | -2.2482521175 |
| H26 | 1.5237891990 | -0.1360143539 | -2.5468336092 |
| H27 | -0.0882772032 | -0.8758771307 | -2.6549348485 |
| H28 | 0.0854459528 | 0.9000262139 | -2.6937754986 |

4- bipyr- $CH_3$
Gas phase Energy: -813.01999829421 hartrees
Solvation Energy: -813.03509856343 hartrees
Zero Point Energy: 121.829 kcal/mol
Free Energy: -27.971 kcal/mol
final geometry:

| | angstroms | | |
|---|---|---|---|
| atom | x | y | z |
| Pd1 | 0.0171310004 | 1.2820080227 | -2.0483544308 |
| N2 | 0.2385629532 | 1.8273674372 | 0.0393144142 |
| N3 | -1.6598664083 | 2.5395873605 | -1.6966110550 |
| C4 | 1.2529717520 | 1.4137821355 | 0.8031494326 |
| C5 | 1.3690898720 | 1.8057363979 | 2.1360680248 |
| C6 | 0.3947648978 | 2.6499223220 | 2.6678921782 |
| C7 | -0.6596228280 | 3.0776857586 | 1.8620657322 |
| C8 | -0.7133896829 | 2.6444778580 | 0.5320906644 |
| C9 | -1.7793900422 | 3.0270617272 | -0.4320265191 |
| C10 | -2.8626289745 | 3.8396337400 | -0.0821463569 |
| C11 | -3.8280061636 | 4.1532307063 | -1.0336852836 |
| C12 | -3.6927582554 | 3.6471621739 | -2.3244444336 |
| C13 | -2.5921745074 | 2.8449033971 | -2.6109214744 |
| H14 | 1.9594395994 | 0.7620156023 | 0.2919860797 |
| H15 | 2.2025013846 | 1.4568766444 | 2.7367202483 |
| H16 | 0.4525260470 | 2.9760486794 | 3.7021191309 |
| H17 | -1.4177708942 | 3.7363401581 | 2.2692582897 |
| H18 | -2.9540010150 | 4.2227261923 | 0.9269837967 |
| H19 | -4.6719650703 | 4.7822486665 | -0.7678090828 |
| H20 | -4.4200592216 | 3.8643843728 | -3.0990454267 |
| H21 | -2.4335882940 | 2.4240458452 | -3.5974846658 |
| H22 | 1.2585572323 | -1.5403900899 | -2.7458643545 |
| O23 | 1.6749351010 | 0.1645745308 | -2.0364704577 |
| O24 | 1.2554413528 | -1.2190795719 | -1.8306570838 |
| C25 | -0.2538819472 | 0.8912503474 | -4.0333092823 |

| | | | |
|---|---|---|---|
| H26 | -0.3491060194 | 1.8314513426 | -4.5917462496 |
| H27 | 0.6137863062 | 0.3431373973 | -4.4087685624 |
| H28 | -1.1617504240 | 0.2890033621 | -4.1692364508 |

TS1- bipyr- $CH_3$
Gas phase Energy: -812.95523481632 hartrees
Solvation Energy: -812.96427262164 hartrees
Zero Point Energy: 128.193 kcal/mol
Free Energy: -30.425 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1421.04 $cm^{-1}$)
final geometry:

| | angstroms | | |
|---|---|---|---|
| atom | x | y | z |
| Pd1 | 0.2979284085 | 0.0426540994 | -0.1984660628 |
| N2 | 0.1517016562 | 0.0775118305 | 2.0036202374 |
| N3 | 2.4567069616 | 0.0170659903 | 0.5965135872 |
| C4 | -1.0259716054 | 0.1037501825 | 2.6466363598 |
| C5 | -1.1215249863 | 0.1177830478 | 4.0369045938 |
| C6 | 0.0531383666 | 0.1034354592 | 4.7843114467 |
| C7 | 1.2750916837 | 0.0769495124 | 4.1188396619 |
| C8 | 1.3005045854 | 0.0651503942 | 2.7185732887 |
| C9 | 2.5716885797 | 0.0396252342 | 1.9415589385 |
| C10 | 3.8331944914 | 0.0402423624 | 2.5533662145 |
| C11 | 4.9785876139 | 0.0167352893 | 1.7632396043 |
| C12 | 4.8446575000 | -0.0066014208 | 0.3768367882 |
| C13 | 3.5585872533 | -0.0051154041 | -0.1592720886 |
| H14 | -1.9092598422 | 0.1147404797 | 2.0117895087 |
| H15 | -2.0964757084 | 0.1391923635 | 4.5118072528 |
| H16 | 0.0238918517 | 0.1126746856 | 5.8698306437 |
| H17 | 2.1950000039 | 0.0648293690 | 4.6902647504 |
| H18 | 3.9282868787 | 0.0601321319 | 3.6322097586 |
| H19 | 5.9605049934 | 0.0172404575 | 2.2270399440 |
| H20 | 5.7099335132 | -0.0250709838 | -0.2772366710 |
| H21 | 3.3928582396 | -0.0219057698 | -1.2324194692 |
| H22 | -1.3681530824 | 0.0823256899 | -0.6167261348 |
| O23 | -2.6189100118 | 0.1141755620 | -0.8380853582 |
| O24 | -3.2846217882 | 0.1523752623 | 0.2546887786 |
| C25 | 0.4990222030 | 0.0100224042 | -2.2318540591 |
| H26 | 1.5624060877 | -0.0614393356 | -2.4975546347 |
| H27 | -0.0270965500 | -0.8517827783 | -2.6577012148 |
| H28 | 0.0881703463 | 0.9275514431 | -2.6686331805 |

1-bipyr-OAc
Gas phase Energy: -851.25413428759 hartrees
Solvation Energy: -851.26992791928 hartrees
Zero Point Energy: 137.899 kcal/mol

Free Energy: -29.061 kcal/mol

final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.2184810518 | 1.5571955682 | -2.0638091345 |
| N2 | 0.4660191188 | 2.0645573851 | 0.1273216449 |
| N3 | -1.6176915993 | 2.3811503625 | -1.5473698345 |
| C4 | 1.5594294058 | 1.9211626675 | 0.8882183537 |
| C5 | 1.5472260745 | 2.1710856235 | 2.2613042858 |
| C6 | 0.3618356309 | 2.5927884426 | 2.8551841266 |
| C7 | -0.7679510670 | 2.7657446351 | 2.0595776725 |
| C8 | -0.6851063739 | 2.4968772141 | 0.6881750386 |
| C9 | -1.8283627461 | 2.6904171359 | -0.2399782921 |
| C10 | -3.0686839834 | 3.1837726024 | 0.1820681789 |
| C11 | -4.0958537273 | 3.3633072124 | -0.7369243316 |
| C12 | -3.8645305829 | 3.0478304032 | -2.0738933212 |
| C13 | -2.6144080379 | 2.5597615309 | -2.4353316554 |
| H14 | 2.4568967092 | 1.6360518295 | 0.3478637437 |
| H15 | 2.4548689084 | 2.0398649693 | 2.8406500283 |
| H16 | 0.3127784291 | 2.7945948447 | 3.9212371894 |
| H17 | -1.6933708504 | 3.1055747900 | 2.5084532832 |
| H18 | -3.2307059255 | 3.4299936533 | 1.2239058391 |
| H19 | -5.0588087698 | 3.7451612159 | -0.4122603828 |
| H20 | -4.6321643008 | 3.1726827744 | -2.8294635642 |
| H21 | -2.3815467035 | 2.2954647631 | -3.4581476342 |
| H22 | -0.1842966546 | 1.2937051988 | -3.5122975673 |
| O23 | 1.8929360408 | 0.5299948651 | -2.6193204975 |
| C24 | 3.0643656444 | 0.9194566006 | -2.2154448700 |
| O25 | 3.3089829759 | 1.8929104334 | -1.4934831910 |
| C26 | 4.1918982792 | 0.0224635408 | -2.7259477300 |
| H27 | 4.2249350673 | 0.0533086804 | -3.8194332868 |
| H28 | 5.1483712824 | 0.3561918450 | -2.3202704861 |
| H29 | 4.0063221394 | -1.0170740724 | -2.4381151271 |

2- bipyr- OAc

Gas phase Energy: -1001.57268434527 hartrees

Solvation Energy: -1001.58784148075 hartrees

Zero Point Energy: 140.467 kcal/mol

Free Energy: -34.922 kcal/mol

final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.2468645813 | -0.2228090472 | -0.1805963892 |
| N2 | 0.1890138386 | 0.0037697009 | 1.8866770496 |
| N3 | 2.3956327774 | 0.2347802011 | 0.3632474355 |
| C4 | -0.9533950184 | -0.0727835630 | 2.5965573761 |

| | | | |
|---|---|---|---|
| C5 | -0.9824545591 | 0.0176662694 | 3.9837358752 |
| C6 | 0.2197952082 | 0.1942060567 | 4.6655139404 |
| C7 | 1.4003796167 | 0.2777440058 | 3.9355104335 |
| C8 | 1.3694293664 | 0.1804542492 | 2.5390647976 |
| C9 | 2.5908459075 | 0.2792001402 | 1.7003313325 |
| C10 | 3.8734559093 | 0.4315910730 | 2.2403983690 |
| C11 | 4.9623760280 | 0.5506887166 | 1.3796721365 |
| C12 | 4.7443019127 | 0.5303628674 | 0.0050711616 |
| C13 | 3.4394098848 | 0.3741144817 | -0.4660763519 |
| H14 | -1.8566561146 | -0.2136317626 | 2.0181592465 |
| H15 | -1.9295864030 | -0.0508433005 | 4.5067610462 |
| H16 | 0.2409311258 | 0.2682735909 | 5.7480775963 |
| H17 | 2.3414557623 | 0.4219495147 | 4.4505735462 |
| H18 | 4.0304160263 | 0.4564271941 | 3.3116915004 |
| H19 | 5.9637855114 | 0.6658390591 | 1.7831535261 |
| H20 | 5.5620118864 | 0.6366551905 | -0.6992891070 |
| H21 | 3.1826637476 | 0.3934205321 | -1.5209293244 |
| H22 | -1.2413549728 | -0.5330477091 | -0.2985817521 |
| O23 | -4.1162301160 | -0.9390228361 | -0.3691879925 |
| O24 | -4.2045824980 | -0.6975811498 | 0.8172841796 |
| O25 | 0.2172793849 | -0.6832815346 | -2.1696999655 |
| C26 | 0.9077087440 | 0.0162743766 | -3.0184130954 |
| O27 | 1.6479969978 | 0.9714352121 | -2.7574682292 |
| C28 | 0.7246664411 | -0.4633894583 | -4.4573380804 |
| H29 | -0.3163080462 | -0.3195730299 | -4.7633863786 |
| H30 | 1.3825335571 | 0.0943067916 | -5.1257376484 |
| H31 | 0.9363681176 | -1.5343235663 | -4.5282619083 |

3A- bipyr- OAc
Gas phase Energy: -1001.60016324321 hartrees
Solvation Energy: -1001.61227060324 hartrees
Zero Point Energy: 142.401 kcal/mol
Free Energy: -32.893 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | -0.3318327111 | 1.0513152339 | -1.8021026614 |
| N2 | 0.1595966654 | 1.9013724140 | 0.1783552569 |
| N3 | -1.8976957676 | 2.6133687302 | -1.4064502162 |
| C4 | 1.2039915870 | 1.4942608946 | 0.9129322268 |
| C5 | 1.5015397568 | 2.0379729659 | 2.1597036628 |
| C6 | 0.6748006252 | 3.0449985026 | 2.6551353956 |
| C7 | -0.4100016767 | 3.4686189008 | 1.8931882971 |
| C8 | -0.6509943132 | 2.8773437556 | 0.6456743170 |
| C9 | -1.7887045473 | 3.2722977575 | -0.2322399454 |
| C10 | -2.7062580760 | 4.2688015282 | 0.1194814661 |

| | | | |
|---|---|---|---|
| C11 | -3.7430142732 | 4.5803428568 | -0.7572887263 |
| C12 | -3.8407896670 | 3.8918427041 | -1.9629468050 |
| C13 | -2.8935103746 | 2.9087506950 | -2.2544809439 |
| H14 | 1.8098245089 | 0.7073366202 | 0.4734460629 |
| H15 | 2.3573188292 | 1.6783434817 | 2.7207920888 |
| H16 | 0.8700030533 | 3.4968672759 | 3.6230506858 |
| H17 | -1.0582139332 | 4.2503789846 | 2.2698011958 |
| H18 | -2.6205018094 | 4.7987925340 | 1.0605908270 |
| H19 | -4.4616248987 | 5.3518342211 | -0.4963973940 |
| H20 | -4.6328893451 | 4.1041423688 | -2.6731119454 |
| H21 | -2.9038449238 | 2.3276597199 | -3.1768927007 |
| H22 | 0.5215763803 | -0.7663749715 | -3.5396761926 |
| O23 | 1.3673336230 | -0.4369880117 | -1.9053143295 |
| O24 | 1.3704305195 | -1.1513032502 | -3.0287506219 |
| O25 | -0.6147966984 | 0.0528607253 | -3.7452828610 |
| C26 | -1.5109217889 | 0.1901890506 | -4.6876625521 |
| O27 | -2.4425510764 | 0.9908121836 | -4.6508005776 |
| C28 | -1.3199362974 | -0.7407585369 | -5.8802502220 |
| H29 | -1.3532804263 | -1.7845529089 | -5.5505551729 |
| H30 | -2.1002658497 | -0.5665680804 | -6.6218796406 |
| H31 | -0.3375884200 | -0.5726974743 | -6.3341919963 |

4- bipyr- OAc
Gas phase Energy: -1001.62289065933 hartrees
Solvation Energy: -1001.64107459276 hartrees
Zero Point Energy: 144.436 kcal/mol
Free Energy: -30.236 kcal/mol
final geometry:

| | angstroms | | |
|---|---|---|---|
| atom | x | y | z |
| Pd1 | -0.2337726730 | 1.0572927797 | -1.8570495861 |
| N2 | 0.2544868362 | 1.8299828672 | -0.0102163381 |
| N3 | -1.8237677033 | 2.4677347396 | -1.5323894386 |
| C4 | 1.3443359606 | 1.4305147835 | 0.6606270005 |
| C5 | 1.6566252411 | 1.9524617640 | 1.9124918961 |
| C6 | 0.8056556101 | 2.9040136395 | 2.4725093322 |
| C7 | -0.3286052252 | 3.3045497942 | 1.7706160685 |
| C8 | -0.5907824633 | 2.7482769481 | 0.5151105640 |
| C9 | -1.7599358658 | 3.0908799512 | -0.3267909493 |
| C10 | -2.7454767586 | 3.9987482703 | 0.0665915609 |
| C11 | -3.8070452378 | 4.2692510681 | -0.7941969785 |
| C12 | -3.8499075568 | 3.6357937434 | -2.0318595837 |
| C13 | -2.8343077869 | 2.7410873447 | -2.3717637884 |
| H14 | 1.9351877338 | 0.6755187430 | 0.1468223310 |
| H15 | 2.5471823269 | 1.6142187600 | 2.4305564323 |
| H16 | 1.0188839941 | 3.3313053452 | 3.4475718300 |

| | | | |
|---|---|---|---|
| H17 | -0.9981303033 | 4.0421275755 | 2.1963906177 |
| H18 | -2.6888543233 | 4.4896644486 | 1.0308844527 |
| H19 | -4.5815280553 | 4.9710298017 | -0.4995378363 |
| H20 | -4.6494053439 | 3.8282130465 | -2.7389562540 |
| H21 | -2.7676150288 | 2.2501740727 | -3.3406551490 |
| H22 | 0.6040917946 | -1.3307490049 | -2.9678997154 |
| O23 | 1.3764994191 | -0.0743140039 | -1.8285556028 |
| O24 | 0.9881772243 | -1.4293451234 | -2.0721312584 |
| O25 | -0.5950860278 | 0.0459343045 | -3.6330874993 |
| C26 | -1.1103210061 | 0.5236612653 | -4.7297853567 |
| O27 | -1.6906600318 | 1.6054817780 | -4.8494419409 |
| C28 | -0.9289078844 | -0.4029131556 | -5.9287775066 |
| H29 | -1.2555683844 | -1.4173147735 | -5.6815275582 |
| H30 | -1.4928697613 | -0.0252625379 | -6.7828138887 |
| H31 | 0.1333384214 | -0.4563803232 | -6.1902514339 |

TS1- bipyr- OAc
Gas phase Energy: -1001.55369041006 hartrees
Solvation Energy: -1001.56691296007 hartrees
Zero Point Energy: 138.387 kcal/mol
Free Energy: -33.067 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1443.61 $cm^{-1}$)
final geometry:

| | angstroms | | |
|---|---|---|---|
| atom | x | y | z |
| Pd1 | 0.1299791197 | -0.1528119173 | -0.1643188609 |
| N2 | 0.0867567523 | 0.0192088668 | 1.9268394607 |
| N3 | 2.3044949712 | 0.2820625318 | 0.4232503235 |
| C4 | -1.0588279962 | -0.0764018031 | 2.6259175196 |
| C5 | -1.0972118614 | -0.0047391187 | 4.0145747937 |
| C6 | 0.0979752424 | 0.1736737286 | 4.7062873651 |
| C7 | 1.2828673824 | 0.2729810858 | 3.9853900298 |
| C8 | 1.2612771432 | 0.1911358034 | 2.5883330781 |
| C9 | 2.4895044734 | 0.2967894831 | 1.7599611491 |
| C10 | 3.7708014760 | 0.4165995586 | 2.3106012183 |
| C11 | 4.8669560559 | 0.5322876013 | 1.4586256332 |
| C12 | 4.6577761703 | 0.5352741570 | 0.0829798171 |
| C13 | 3.3533492280 | 0.4095424381 | -0.3991767568 |
| H14 | -1.9652441905 | -0.2226072206 | 2.0455900761 |
| H15 | -2.0475847656 | -0.0889958194 | 4.5298040288 |
| H16 | 0.1112531177 | 0.2359139226 | 5.7901008136 |
| H17 | 2.2198486502 | 0.4179420041 | 4.5082718254 |
| H18 | 3.9212785501 | 0.4158170724 | 3.3834368918 |
| H19 | 5.8678494811 | 0.6226722783 | 1.8704897322 |
| H20 | 5.4827749969 | 0.6339031428 | -0.6145111992 |
| H21 | 3.0990337753 | 0.4273335553 | -1.4568381756 |

| | | | |
|---|---|---|---|
| H22 | -1.4891576018 | -0.4694581842 | -0.2962575849 |
| O23 | -2.7726106511 | -0.7420319187 | -0.5293550914 |
| O24 | -3.4611001116 | -0.7113521142 | 0.5296215206 |
| O25 | -0.0388247089 | -0.5505969201 | -2.1525581855 |
| C26 | 0.7515770760 | -0.0651029718 | -3.0645939595 |
| O27 | 1.7226408908 | 0.6725998422 | -2.8733524170 |
| C28 | 0.3709736672 | -0.5112275022 | -4.4737407212 |
| H29 | -0.6609814476 | -0.2218696332 | -4.6935448718 |
| H30 | 1.0464557430 | -0.0635728363 | -5.2042578186 |
| H31 | 0.4216822173 | -1.6025725071 | -4.5432522173 |

1-bipyr-I
Gas phase Energy: -634.19958772809 hartrees
Solvation Energy: -634.21353328785 hartrees
Zero Point Energy: 106.044 kcal/mol
Free Energy: -26.805 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | -0.0339527609 | 1.1821714174 | -1.8592243263 |
| N2 | 0.1743510240 | 1.8392485222 | 0.1464455259 |
| N3 | -1.7278128512 | 2.6134099809 | -1.5981674728 |
| C4 | 1.1451356395 | 1.4173907203 | 0.9750208400 |
| C5 | 1.2598402141 | 1.8634345931 | 2.2876001413 |
| C6 | 0.3291098658 | 2.7855873273 | 2.7610279399 |
| C7 | -0.6771374559 | 3.2249309811 | 1.9072200035 |
| C8 | -0.7400163890 | 2.7387604961 | 0.5957260468 |
| C9 | -1.7891299491 | 3.1675432250 | -0.3670279058 |
| C10 | -2.7925141409 | 4.0893241088 | -0.0419902776 |
| C11 | -3.7362962917 | 4.4349291290 | -1.0057415741 |
| C12 | -3.6601622982 | 3.8557540209 | -2.2703252720 |
| C13 | -2.6346479238 | 2.9458390969 | -2.5236938707 |
| H14 | 1.8407810046 | 0.7014821259 | 0.5554870620 |
| H15 | 2.0619356932 | 1.4917343605 | 2.9156000567 |
| H16 | 0.3831012101 | 3.1588985661 | 3.7789241734 |
| H17 | -1.4074944474 | 3.9413787669 | 2.2620584541 |
| H18 | -2.8443153077 | 4.5354039504 | 0.9437168899 |
| H19 | -4.5197950850 | 5.1483039679 | -0.7677548414 |
| H20 | -4.3759700223 | 4.0987146005 | -3.0481360758 |
| H21 | -2.5165505523 | 2.4570034777 | -3.4871460805 |
| H22 | 1.1573463789 | 0.2348074445 | -1.9041039361 |
| I25 | -0.3241128424 | 0.3838962797 | -4.3651508298 |

2- bipyr- I
Gas phase Energy: -784.51806729102 hartrees
Solvation Energy: -784.53163227954 hartrees

Zero Point Energy: 108.657 kcal/mol
Free Energy: -32.209 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.4428524336 | 0.0381702997 | -0.0808743135 |
| N2 | 0.2051048392 | 0.0566296067 | 2.0300703371 |
| N3 | 2.5384260452 | 0.0048343439 | 0.6827122941 |
| C4 | -0.9879913720 | 0.0822949694 | 2.6494890837 |
| C5 | -1.1154012546 | 0.0933028927 | 4.0351728515 |
| C6 | 0.0423764574 | 0.0771474623 | 4.8100452103 |
| C7 | 1.2787528343 | 0.0506727546 | 4.1725339819 |
| C8 | 1.3427961774 | 0.0406332797 | 2.7740250453 |
| C9 | 2.6306678874 | 0.0122254158 | 2.0311974412 |
| C10 | 3.8797828362 | -0.0062327784 | 2.6646786086 |
| C11 | 5.0364744070 | -0.0324910100 | 1.8890098361 |
| C12 | 4.9248522932 | -0.0397873402 | 0.5001890660 |
| C13 | 3.6494645972 | -0.0203730956 | -0.0626234393 |
| H14 | -1.8551806367 | 0.0940699396 | 2.0014481748 |
| H15 | -2.1013381095 | 0.1140202660 | 4.4855937298 |
| H16 | -0.0123690368 | 0.0849343283 | 5.8939573646 |
| H17 | 2.1863962933 | 0.0378557757 | 4.7627519116 |
| H18 | 3.9585456932 | -0.0003744957 | 3.7447785409 |
| H19 | 6.0107391578 | -0.0470031445 | 2.3676109383 |
| H20 | 5.8004862253 | -0.0600065157 | -0.1390709396 |
| H21 | 3.4882666631 | -0.0247096603 | -1.1372982490 |
| H22 | -1.0281227831 | 0.0624772494 | -0.4695476946 |
| O23 | -3.8709416101 | 0.0781666198 | -0.4901953898 |
| O24 | -4.1081164456 | 0.1173667140 | 0.7001748702 |
| I25 | 0.7700208908 | 0.0142531168 | -2.7067363270 |

3A- bipyr- I
Gas phase Energy: -784.52881051369 hartrees
Solvation Energy: -784.54157319077 hartrees
Zero Point Energy: 110.928 kcal/mol
Free Energy: -29.768 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | -0.0701479427 | 1.1946965055 | -1.8086480662 |
| N2 | 0.1785760303 | 1.9419038740 | 0.3010633120 |
| N3 | -1.7355487976 | 2.6671003611 | -1.4604366792 |
| C4 | 1.1497045524 | 1.5256864232 | 1.1228973264 |
| C5 | 1.2736378175 | 1.9866857355 | 2.4315604930 |
| C6 | 0.3444676285 | 2.9165495102 | 2.8934800737 |
| C7 | -0.6654968212 | 3.3489445694 | 2.0387274237 |

| | | | |
|---|---|---|---|
| C8 | -0.7289584152 | 2.8432168157 | 0.7334477524 |
| C9 | -1.7782596918 | 3.2531105172 | -0.2434570099 |
| C10 | -2.7683374352 | 4.1950347279 | 0.0619328933 |
| C11 | -3.7184554896 | 4.5261248635 | -0.9003487536 |
| C12 | -3.6624269067 | 3.9119247729 | -2.1488339556 |
| C13 | -2.6488952624 | 2.9849542579 | -2.3866226968 |
| H14 | 1.8404899446 | 0.7997453619 | 0.7035968713 |
| H15 | 2.0760570106 | 1.6229374483 | 3.0643723173 |
| H16 | 0.4017224708 | 3.3021817376 | 3.9070333881 |
| H17 | -1.3932637619 | 4.0696767893 | 2.3913444513 |
| H18 | -2.8031694770 | 4.6695152493 | 1.0351713179 |
| H19 | -4.4905838883 | 5.2553627834 | -0.6735853146 |
| H20 | -4.3829572458 | 4.1403322669 | -2.9267665953 |
| H21 | -2.5468283972 | 2.4709760150 | -3.3382440289 |
| H22 | 1.3992847754 | -0.7017433791 | -3.3613965638 |
| O23 | 1.6546460553 | -0.1013954033 | -1.6213856323 |
| O24 | 2.0535201550 | -0.8938255874 | -2.6248417644 |
| I25 | -0.5341171564 | 0.3681747274 | -4.4673731592 |

4- bipyr- I
Gas phase Energy: -784.55779703219 hartrees
Solvation Energy: -784.5755579535 hartrees
Zero Point Energy: 112.309 kcal/mol
Free Energy: -28.454 kcal/mol
final geometry:

| | angstroms | | |
|---|---|---|---|
| atom | x | y | z |
| Pd1 | 0.0279129344 | 1.2832021177 | -1.8708866363 |
| N2 | 0.2292475596 | 1.8300096688 | 0.1461891749 |
| N3 | -1.6633886955 | 2.5580066922 | -1.5838813944 |
| C4 | 1.2312643036 | 1.3944583512 | 0.9180304621 |
| C5 | 1.3295909205 | 1.7632251337 | 2.2574740945 |
| C6 | 0.3528433790 | 2.6015572045 | 2.7922799932 |
| C7 | -0.6863753817 | 3.0488458008 | 1.9788167018 |
| C8 | -0.7286965097 | 2.6467910730 | 0.6401851467 |
| C9 | -1.7786708439 | 3.0561612982 | -0.3244931522 |
| C10 | -2.8369819254 | 3.9036399986 | 0.0147432370 |
| C11 | -3.7824793311 | 4.2408774475 | -0.9499435864 |
| C12 | -3.6500248384 | 3.7245435724 | -2.2359687408 |
| C13 | -2.5736063515 | 2.8844331779 | -2.5125937589 |
| H14 | 1.9388027862 | 0.7437227703 | 0.4090188219 |
| H15 | 2.1533472093 | 1.3972892292 | 2.8605669201 |
| H16 | 0.3959279823 | 2.9067429412 | 3.8333892797 |
| H17 | -1.4503124725 | 3.7001417719 | 2.3862460787 |
| H18 | -2.9240102130 | 4.2972137067 | 1.0203538875 |
| H19 | -4.6086267324 | 4.8981049746 | -0.6964102633 |

| | | | |
|---|---|---|---|
| H20 | -4.3618319504 | 3.9613832620 | -3.0190039520 |
| H21 | -2.4135924658 | 2.4487485071 | -3.4938685850 |
| H22 | 1.1937755816 | -1.3487181098 | -2.7218495677 |
| O23 | 1.6642140565 | 0.1983807135 | -1.7684187833 |
| O24 | 1.2722911021 | -1.1780292610 | -1.7650210524 |
| I25 | -0.2773952425 | 0.6699415056 | -4.4954604500 |

TS1- bipyr- I
Gas phase Energy: -784.49488553333 hartrees
Solvation Energy: -784.50756124424 hartrees
Zero Point Energy: 106.488 kcal/mol
Free Energy: -31.109 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1621.62 $cm^{-1}$)
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.3410854364 | 0.0424610864 | -0.0428536013 |
| N2 | 0.1703112447 | 0.0628444697 | 2.0862809298 |
| N3 | 2.4650903067 | 0.0113784707 | 0.6742156327 |
| C4 | -1.0041267442 | 0.0881322958 | 2.7365770178 |
| C5 | -1.0915746583 | 0.0982345025 | 4.1262198570 |
| C6 | 0.0862831355 | 0.0813870353 | 4.8681471350 |
| C7 | 1.3040880023 | 0.0553998344 | 4.1958241813 |
| C8 | 1.3276474407 | 0.0465097846 | 2.7966516421 |
| C9 | 2.5932941726 | 0.0192588811 | 2.0179492175 |
| C10 | 3.8594668097 | 0.0022698709 | 2.6165521709 |
| C11 | 4.9941738818 | -0.0232416895 | 1.8101083959 |
| C12 | 4.8439206121 | -0.0312245547 | 0.4253239041 |
| C13 | 3.5537136430 | -0.0131141677 | -0.1022938982 |
| H14 | -1.8936516219 | 0.1005467160 | 2.1127845629 |
| H15 | -2.0648605156 | 0.1187641450 | 4.6039366621 |
| H16 | 0.0622374336 | 0.0882865723 | 5.9535747192 |
| H17 | 2.2283880078 | 0.0420168830 | 4.7600474414 |
| H18 | 3.9672166860 | 0.0087764478 | 3.6944131773 |
| H19 | 5.9815717111 | -0.0366347965 | 2.2618393949 |
| H20 | 5.7019487487 | -0.0509571548 | -0.2378256574 |
| H21 | 3.3647946640 | -0.0179842758 | -1.1719904700 |
| H22 | -1.3112221082 | 0.0667899634 | -0.4027017397 |
| O23 | -2.5908938778 | 0.0824209925 | -0.6144510230 |
| O24 | -3.2682782280 | 0.1113842018 | 0.4517886151 |
| I25 | 0.5626800339 | 0.0148827888 | -2.6887203983 |

1-bipyr-CN
Gas phase Energy: -715.61340084282 hartrees
Solvation Energy: -715.63220142774 hartrees
Zero Point Energy: 110.745 kcal/mol

Free Energy: -25.849 kcal/mol

final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.0084687031 | 1.1603447042 | -2.0293832210 |
| N2 | 0.2295090101 | 1.7895243370 | 0.0015746675 |
| N3 | -1.6584565262 | 2.5709350055 | -1.7425285956 |
| C4 | 1.1996126447 | 1.3608324562 | 0.8237880951 |
| C5 | 1.3148515026 | 1.7936476589 | 2.1413756952 |
| C6 | 0.3827758422 | 2.7099866810 | 2.6220305958 |
| C7 | -0.6255496939 | 3.1574335530 | 1.7732236371 |
| C8 | -0.6863200680 | 2.6823014070 | 0.4580898848 |
| C9 | -1.7344551483 | 3.1132274948 | -0.5072549067 |
| C10 | -2.7497621835 | 4.0212023035 | -0.1863605330 |
| C11 | -3.6873801813 | 4.3641494015 | -1.1579392284 |
| C12 | -3.5940228157 | 3.7964552066 | -2.4264930483 |
| C13 | -2.5577826143 | 2.8982427455 | -2.6786589587 |
| H14 | 1.8957515025 | 0.6496961075 | 0.3955855425 |
| H15 | 2.1173980272 | 1.4170444023 | 2.7658091589 |
| H16 | 0.4372891604 | 3.0734613278 | 3.6435223643 |
| H17 | -1.3561522266 | 3.8701434200 | 2.1349774417 |
| H18 | -2.8158868680 | 4.4577480852 | 0.8029168849 |
| H19 | -4.4804259870 | 5.0673526241 | -0.9219524087 |
| H20 | -4.3052412550 | 4.0388432191 | -3.2085515304 |
| H21 | -2.4241499896 | 2.4170168303 | -3.6432886090 |
| H22 | 1.1907147781 | 0.1860840346 | -2.1607825251 |
| C25 | -0.3074690247 | 0.6718873326 | -3.8887203645 |
| N26 | -0.6304315074 | 0.4852995546 | -4.9974890288 |

2- bipyr- CN

Gas phase Energy: -865.93197230595 hartrees

Solvation Energy: -865.9501548506 hartrees

Zero Point Energy: 113.365 kcal/mol

Free Energy: -31.336 kcal/mol

final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.4551423948 | 0.0547166565 | -0.2041147974 |
| N2 | 0.2151303895 | 0.0743144347 | 1.9223331259 |
| N3 | 2.5234314823 | 0.0235549034 | 0.5469417913 |
| C4 | -0.9719103986 | 0.1008185940 | 2.5492610630 |
| C5 | -1.0879772428 | 0.1160352707 | 3.9365827665 |
| C6 | 0.0772741669 | 0.1033046107 | 4.6997429828 |
| C7 | 1.3098398419 | 0.0753284057 | 4.0530364788 |
| C8 | 1.3594912528 | 0.0607980946 | 2.6546495513 |
| C9 | 2.6383848982 | 0.0303393404 | 1.8933915392 |

| | | | |
|---|---|---|---|
| C10 | 3.8990839400 | 0.0090999154 | 2.5012344811 |
| C11 | 5.0397178238 | -0.0186942910 | 1.7006996143 |
| C12 | 4.9022658678 | -0.0247374710 | 0.3140704217 |
| C13 | 3.6167800958 | -0.0030186829 | -0.2256870526 |
| H14 | -1.8430863286 | 0.1095152211 | 1.9054522486 |
| H15 | -2.0694794453 | 0.1374501807 | 4.3963358090 |
| H16 | 0.0314386070 | 0.1148801922 | 5.7840001062 |
| H17 | 2.2226732877 | 0.0653596238 | 4.6353542988 |
| H18 | 3.9992179366 | 0.0135521121 | 3.5796849972 |
| H19 | 6.0233493569 | -0.0354836005 | 2.1595133181 |
| H20 | 5.7657374098 | -0.0460230672 | -0.3413804823 |
| H21 | 3.4316970286 | -0.0065897822 | -1.2960328586 |
| H22 | -1.0104886795 | 0.0759827092 | -0.6635352525 |
| O23 | -3.8214516264 | 0.0946653421 | -0.8510275114 |
| O24 | -4.0575158967 | 0.0981976612 | 0.3400086275 |
| C25 | 0.8136817118 | 0.0351725672 | -2.1197109511 |
| N26 | 1.1906790108 | 0.0212160985 | -3.2272520499 |

3A- bipyr- CN
Gas phase Energy: -865.93241744829 hartrees
Solvation Energy: -865.94736498004 hartrees
Zero Point Energy: 115.161 kcal/mol
Free Energy: -29.246 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | -0.1581612929 | 1.1804868955 | -2.0006511347 |
| N2 | 0.1056215605 | 1.9086967988 | 0.0705924543 |
| N3 | -1.8446771316 | 2.6830971754 | -1.6102639394 |
| C4 | 1.0931714349 | 1.4670035498 | 0.8620426129 |
| C5 | 1.2572371652 | 1.9031588406 | 2.1745440511 |
| C6 | 0.3530185872 | 2.8351670146 | 2.6789846345 |
| C7 | -0.6738526011 | 3.2951383187 | 1.8592828712 |
| C8 | -0.7779842014 | 2.8152485705 | 0.5475420727 |
| C9 | -1.8468033007 | 3.2601115383 | -0.3919957303 |
| C10 | -2.8093462139 | 4.2207679634 | -0.0562653911 |
| C11 | -3.7735082490 | 4.5756443951 | -0.9964277005 |
| C12 | -3.7585980895 | 3.9683607393 | -2.2503542572 |
| C13 | -2.7685226211 | 3.0231208048 | -2.5138177698 |
| H14 | 1.7662946629 | 0.7413371462 | 0.4151142972 |
| H15 | 2.0723189060 | 1.5180278113 | 2.7776036127 |
| H16 | 0.4425715802 | 3.2006988650 | 3.6975375067 |
| H17 | -1.3844673415 | 4.0170634589 | 2.2427615052 |
| H18 | -2.8119926800 | 4.6915495263 | 0.9196121931 |
| H19 | -4.5254180698 | 5.3190499750 | -0.7493567932 |
| H20 | -4.4920367006 | 4.2171917352 | -3.0097566018 |

| | | | |
|---|---|---|---|
| H21 | -2.6979786171 | 2.5142534516 | -3.4706055170 |
| H22 | 1.3641630694 | -0.7514490752 | -3.6745702651 |
| O23 | 1.7583337582 | -0.2666973941 | -1.9103352639 |
| O24 | 2.0678013313 | -0.9871028287 | -2.9783029046 |
| C25 | -0.2891812904 | 0.4325832770 | -3.8875918686 |
| N26 | 0.0359207439 | -0.2299588492 | -4.8022753501 |

4- bipyr- CN
Gas phase Energy: -865.96937589850 hartrees
Solvation Energy: -865.99211789692 hartrees
Zero Point Energy: 116.918 kcal/mol
Free Energy: -27.831 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.0143671643 | 1.2553662916 | -2.0194089288 |
| N2 | 0.2358647989 | 1.8079301596 | -0.0006756724 |
| N3 | -1.6473253883 | 2.5284267491 | -1.7337758390 |
| C4 | 1.2303149274 | 1.3627108044 | 0.7736249933 |
| C5 | 1.3385339704 | 1.7462969470 | 2.1090318706 |
| C6 | 0.3764626171 | 2.6081075864 | 2.6334714785 |
| C7 | -0.6601844836 | 3.0627880280 | 1.8185206949 |
| C8 | -0.7101130832 | 2.6439925609 | 0.4857548986 |
| C9 | -1.7598003343 | 3.0486690467 | -0.4839758515 |
| C10 | -2.8172666365 | 3.9042203444 | -0.1656157448 |
| C11 | -3.7601433755 | 4.2204054255 | -1.1410245911 |
| C12 | -3.6283221639 | 3.6775133549 | -2.4167146590 |
| C13 | -2.5521137934 | 2.8321463278 | -2.6758533144 |
| H14 | 1.9226220295 | 0.6908340072 | 0.2697067559 |
| H15 | 2.1565324479 | 1.3739612009 | 2.7156848941 |
| H16 | 0.4279097367 | 2.9255466074 | 3.6704174201 |
| H17 | -1.4131404634 | 3.7300334523 | 2.2202786304 |
| H18 | -2.9068663343 | 4.3192846686 | 0.8312088961 |
| H19 | -4.5862952254 | 4.8832684504 | -0.9032890186 |
| H20 | -4.3402967958 | 3.8985630962 | -3.2040424151 |
| H21 | -2.3869767723 | 2.3754137375 | -3.6462489369 |
| H22 | 1.2981719849 | -1.3277392953 | -3.0826390635 |
| O23 | 1.6528613339 | 0.1430528981 | -1.9607449038 |
| O24 | 1.2846430882 | -1.2405042546 | -2.1141789961 |
| C25 | -0.3049176130 | 0.8489799130 | -3.9278275779 |
| N26 | -0.5798596222 | 0.6459944764 | -5.0462863880 |

TS1- bipyr- CN
Gas phase Energy: -865.90675257034 hartrees
Solvation Energy: -865.92429262198 hartrees
Zero Point Energy: 111.320 kcal/mol

Free Energy: -29.728 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1561.08 $cm^{-1}$)
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.3078741688 | 0.0516909067 | -0.1791834281 |
| N2 | 0.1290484609 | 0.0705264470 | 1.9558056849 |
| N3 | 2.4125604750 | 0.0238774166 | 0.5359311858 |
| C4 | -1.0455549219 | 0.0938038183 | 2.6037356211 |
| C5 | -1.1320890496 | 0.1106601584 | 3.9939157118 |
| C6 | 0.0474040565 | 0.1041473012 | 4.7334492145 |
| C7 | 1.2666238619 | 0.0799078993 | 4.0617868107 |
| C8 | 1.2873089350 | 0.0621167972 | 2.6635180114 |
| C9 | 2.5510792547 | 0.0331334844 | 1.8778232932 |
| C10 | 3.8231791440 | 0.0145806176 | 2.4616686025 |
| C11 | 4.9480889296 | -0.0130363171 | 1.6401615135 |
| C12 | 4.7840043225 | -0.0217401922 | 0.2567923510 |
| C13 | 3.4883154486 | -0.0025676698 | -0.2576964724 |
| H14 | -1.9330401390 | 0.0990499768 | 1.9758095714 |
| H15 | -2.1044136824 | 0.1289924274 | 4.4736030680 |
| H16 | 0.0234391671 | 0.1177923505 | 5.8188173956 |
| H17 | 2.1923034063 | 0.0757512019 | 4.6240924244 |
| H18 | 3.9434951169 | 0.0206607780 | 3.5383481816 |
| H19 | 5.9406334901 | -0.0278154531 | 2.0802197430 |
| H20 | 5.6352050889 | -0.0431434617 | -0.4150085652 |
| H21 | 3.2836348887 | -0.0081620536 | -1.3245349215 |
| H22 | -1.3449518906 | 0.0759945262 | -0.6431753887 |
| O23 | -2.5959504675 | 0.0982558740 | -0.8643182525 |
| O24 | -3.2727464610 | 0.1055695866 | 0.2084065945 |
| C25 | 0.6077181162 | 0.0334980828 | -2.1177521171 |
| N26 | 0.9438873857 | 0.0206873880 | -3.2385365978 |

1-bipyr-$CF_3$
Gas phase Energy: -960.38780971527 hartrees
Solvation Energy: -960.39918936176 hartrees
Zero Point Energy: 114.009 kcal/mol
Free Energy: -27.008 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | -0.0071116694 | 1.1917137833 | -2.0404505618 |
| N2 | 0.1728947509 | 1.8222750830 | 0.0254944984 |
| N3 | -1.7130187408 | 2.6443543444 | -1.7095814895 |
| C4 | 1.1494093111 | 1.3803610211 | 0.8308987177 |
| C5 | 1.2829063682 | 1.7998384976 | 2.1516567944 |
| C6 | 0.3611684445 | 2.7182820143 | 2.6489547691 |

| | | | |
|---|---|---|---|
| C7 | -0.6539787335 | 3.1788334146 | 1.8154792863 |
| C8 | -0.7305209126 | 2.7118651771 | 0.4970391975 |
| C9 | -1.7859034742 | 3.1505813073 | -0.4568761572 |
| C10 | -2.8084315396 | 4.0356509837 | -0.0932953179 |
| C11 | -3.7639803008 | 4.4024075981 | -1.0371219078 |
| C12 | -3.6781887356 | 3.8766014236 | -2.3229156494 |
| C13 | -2.6348723563 | 2.9990785315 | -2.6149974911 |
| H14 | 1.8352072162 | 0.6694145842 | 0.3848846563 |
| H15 | 2.0898020970 | 1.4134625527 | 2.7643796591 |
| H16 | 0.4291715979 | 3.0743031102 | 3.6723108049 |
| H17 | -1.3733326809 | 3.8954049012 | 2.1917740439 |
| H18 | -2.8667643194 | 4.4343110109 | 0.9117694641 |
| H19 | -4.5620374782 | 5.0875288356 | -0.7669309862 |
| H20 | -4.4005914882 | 4.1338240614 | -3.0901505180 |
| H21 | -2.5135145824 | 2.5545543721 | -3.5949224716 |
| H22 | 1.1869763504 | 0.2122762359 | -2.0906904011 |
| C23 | -0.1586066878 | 0.6101462573 | -3.9495016492 |
| F24 | -1.1863735335 | 1.2883803383 | -4.6029760334 |
| F25 | 0.9373702402 | 0.8512959030 | -4.7178839293 |
| F26 | -0.4646661228 | -0.7048881410 | -4.1217958707 |

2- bipyr- $CF_3$
Gas phase Energy: -1110.70635125832 hartrees
Solvation Energy: -1110.71695542013 hartrees
Zero Point Energy: 116.641 kcal/mol
Free Energy: -33.567 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.4624901300 | 0.0444583831 | -0.2371471873 |
| N2 | 0.2512074536 | 0.0714626411 | 1.9317564542 |
| N3 | 2.5770926869 | 0.0176070209 | 0.5766060967 |
| C4 | -0.9427106879 | 0.1016940530 | 2.5433133827 |
| C5 | -1.0772112681 | 0.1244474178 | 3.9294342210 |
| C6 | 0.0787638034 | 0.1162026907 | 4.7068743452 |
| C7 | 1.3186282712 | 0.0854055001 | 4.0752311220 |
| C8 | 1.3819252163 | 0.0628577671 | 2.6759889782 |
| C9 | 2.6674926614 | 0.0282156736 | 1.9268621077 |
| C10 | 3.9136127847 | 0.0065171901 | 2.5662057212 |
| C11 | 5.0760406640 | -0.0268014757 | 1.8000487878 |
| C12 | 4.9699859573 | -0.0379013181 | 0.4119607042 |
| C13 | 3.6974563794 | -0.0147061055 | -0.1578019568 |
| H14 | -1.8052931770 | 0.1078428706 | 1.8878031251 |
| H15 | -2.0640371983 | 0.1481846702 | 4.3778588722 |
| H16 | 0.0202580499 | 0.1335500207 | 5.7906277729 |
| H17 | 2.2231612716 | 0.0795799821 | 4.6704369955 |

| | | | |
|---|---|---|---|
| H18 | 3.9841519732 | 0.0142600820 | 3.6468513969 |
| H19 | 6.0472117271 | -0.0441695498 | 2.2850725657 |
| H20 | 5.8476484956 | -0.0641104788 | -0.2242387165 |
| H21 | 3.5442442729 | -0.0212883792 | -1.2297633788 |
| H22 | -1.0322185773 | 0.0630498676 | -0.6167971026 |
| O23 | -3.8930140625 | 0.0894583302 | -0.6688404462 |
| O24 | -4.0662241824 | 0.0741915597 | 0.5328304234 |
| C25 | 0.6404201330 | 0.0218194332 | -2.2353516663 |
| F26 | 1.9804084618 | 0.0244528353 | -2.6260774958 |
| F27 | 0.1200024897 | -1.0781352863 | -2.8452903343 |
| F28 | 0.1061511314 | 1.0980699931 | -2.8751394666 |

3A- bipyr- $CF_3$
Gas phase Energy: -1110.69909006223 hartrees
Solvation Energy: -1110.70864744169 hartrees
Zero Point Energy: 118.870 kcal/mol
Free Energy: -32.080 kcal/mol
final geometry:

| | angstroms | | |
|---|---|---|---|
| atom | x | y | z |
| Pd1 | -0.0411522195 | 1.1924140265 | -2.0114712259 |
| N2 | 0.2023805130 | 1.9462554207 | 0.0869182974 |
| N3 | -1.9400778623 | 2.4502015165 | -1.5102319075 |
| C4 | 1.1749689152 | 1.5183042968 | 0.9046506790 |
| C5 | 1.2358046307 | 1.8668723611 | 2.2513214764 |
| C6 | 0.2305792359 | 2.6808451120 | 2.7709279253 |
| C7 | -0.7886149818 | 3.1152528867 | 1.9294023649 |
| C8 | -0.7758797991 | 2.7396708129 | 0.5797996046 |
| C9 | -1.8315877118 | 3.1703893765 | -0.3736446682 |
| C10 | -2.6752593909 | 4.2607543661 | -0.1229934994 |
| C11 | -3.6655523721 | 4.5799450630 | -1.0476924544 |
| C12 | -3.7842710446 | 3.8124714886 | -2.2061065273 |
| C13 | -2.8890057003 | 2.7633615219 | -2.4019651526 |
| H14 | 1.9176069516 | 0.8689852471 | 0.4514612783 |
| H15 | 2.0473317535 | 1.5006948809 | 2.8707597335 |
| H16 | 0.2314774269 | 2.9642728921 | 3.8191219055 |
| H17 | -1.5982612178 | 3.7192280198 | 2.3220190555 |
| H18 | -2.5494723460 | 4.8628731533 | 0.7697041969 |
| H19 | -4.3283584521 | 5.4212827843 | -0.8689208318 |
| H20 | -4.5466537535 | 4.0223721040 | -2.9488810648 |
| H21 | -2.9103650045 | 2.1446238290 | -3.2930955717 |
| H22 | 1.2264273938 | -1.1439499465 | -3.2121172444 |
| O23 | 1.6204746142 | -0.2904858930 | -1.6176745073 |
| O24 | 1.8040407581 | -1.3448526819 | -2.4277198401 |
| C25 | -0.3803728763 | 0.6717669682 | -3.9844113087 |
| F26 | -1.7112510050 | 0.5294323992 | -4.3174681803 |

| | | | |
|---|---|---|---|
| F27 | 0.1227303851 | 1.5195397421 | -4.9251608609 |
| F28 | 0.1633222473 | -0.5961291658 | -4.3676801913 |

4- bipyr- $CF_3$
Gas phase Energy: -1110.74885907135 hartrees
Solvation Energy: -1110.76380889272 hartrees
Zero Point Energy: 120.520 kcal/mol
Free Energy: -28.277 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | -0.0134291234 | 1.2420055902 | -2.0415592339 |
| N2 | 0.2006065128 | 1.8136967879 | 0.0030328413 |
| N3 | -1.6990875540 | 2.5588026906 | -1.7186304254 |
| C4 | 1.2049430827 | 1.3656994054 | 0.7617316036 |
| C5 | 1.3252467241 | 1.7362855543 | 2.0994935709 |
| C6 | 0.3670408605 | 2.5914982531 | 2.6405890923 |
| C7 | -0.6748687725 | 3.0542478594 | 1.8380934529 |
| C8 | -0.7350041881 | 2.6454922441 | 0.5019027192 |
| C9 | -1.7855205547 | 3.0687136827 | -0.4611991309 |
| C10 | -2.8155500309 | 3.9481456739 | -0.1161691994 |
| C11 | -3.7634181373 | 4.3094670746 | -1.0691635737 |
| C12 | -3.6618439963 | 3.7823470316 | -2.3527814675 |
| C13 | -2.6145296442 | 2.9087038345 | -2.6349484334 |
| H14 | 1.8966427584 | 0.7063382326 | 0.2403446943 |
| H15 | 2.1496783851 | 1.3601404482 | 2.6953109663 |
| H16 | 0.4267282930 | 2.8993191514 | 3.6800836299 |
| H17 | -1.4221676215 | 3.7195962065 | 2.2534737410 |
| H18 | -2.8776353963 | 4.3501699521 | 0.8875558536 |
| H19 | -4.5658422986 | 4.9928071511 | -0.8086687181 |
| H20 | -4.3756231580 | 4.0350678013 | -3.1291348456 |
| H21 | -2.4880478434 | 2.4610253327 | -3.6120031674 |
| H22 | 1.1441251284 | -1.4541683481 | -2.7590976653 |
| O23 | 1.6609222076 | 0.1639361577 | -1.9555149059 |
| O24 | 1.2933699253 | -1.2300092341 | -1.8253239046 |
| C25 | -0.1864327054 | 0.7593589641 | -3.9855824728 |
| F26 | -1.4805919074 | 0.8568980127 | -4.4725040053 |
| F27 | 0.5552118143 | 1.5584708909 | -4.7978742513 |
| F28 | 0.1839283733 | -0.5272023035 | -4.2935507448 |

TS1- bipyr- $CF_3$
Gas phase Energy: -1110.68137390433 hartrees
Solvation Energy: -1110.69168751477 hartrees
Zero Point Energy: 114.709 kcal/mol
Free Energy: -28.277 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1488.76 $cm^{-1}$)

final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.3211957922 | 0.0489704050 | -0.1974051210 |
| N2 | 0.1773785604 | 0.0682412152 | 1.9742825725 |
| N3 | 2.4868695816 | 0.0008363082 | 0.5706227697 |
| C4 | -1.0034265033 | 0.0990793296 | 2.6104309655 |
| C5 | -1.1038221879 | 0.1208714815 | 3.9997434292 |
| C6 | 0.0690963508 | 0.1104048223 | 4.7491816016 |
| C7 | 1.2940063440 | 0.0772479487 | 4.0888200159 |
| C8 | 1.3262617002 | 0.0557032280 | 2.6896308830 |
| C9 | 2.5995000642 | 0.0167977896 | 1.9155782233 |
| C10 | 3.8587063888 | -0.0046806953 | 2.5293088700 |
| C11 | 5.0043715925 | -0.0454196901 | 1.7388873961 |
| C12 | 4.8714869569 | -0.0638737222 | 0.3531563195 |
| C13 | 3.5873820062 | -0.0376962892 | -0.1889512518 |
| H14 | -1.8855080032 | 0.1059683747 | 1.9741689340 |
| H15 | -2.0803680254 | 0.1456249157 | 4.4705744991 |
| H16 | 0.0363773485 | 0.1274895842 | 5.8343024436 |
| H17 | 2.2116817660 | 0.0681019578 | 4.6632837952 |
| H18 | 3.9531215334 | 0.0101509998 | 3.6082749099 |
| H19 | 5.9856876362 | -0.0622836319 | 2.2036592250 |
| H20 | 5.7369582295 | -0.0956431226 | -0.3000324209 |
| H21 | 3.4129353932 | -0.0412591386 | -1.2588809563 |
| H22 | -1.3624029327 | 0.0910494375 | -0.5780162620 |
| O23 | -2.5924776653 | 0.1761745673 | -0.8274488196 |
| O24 | -3.2850767471 | 0.1464463084 | 0.2441553443 |
| C25 | 0.4970408971 | 0.0165592153 | -2.1868240771 |
| F26 | 1.7563615467 | 0.4292106080 | -2.5953104480 |
| F27 | 0.3471418259 | -1.2336704659 | -2.7192369305 |
| F28 | -0.3696043567 | 0.8230877672 | -2.8639631796 |

1-bipyr-Cl- LACV3P**++
Gas phase Energy: -1083.15439968845 hartrees
Zero Point Energy: 105.674 kcal/mol
Free Energy: -24.048 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.1036702961 | 1.3810867178 | -2.0375120881 |
| N2 | 0.4198653768 | 1.9029528081 | 0.0862351379 |
| N3 | -1.6624760721 | 2.3729738205 | -1.5309169944 |
| C4 | 1.5067855021 | 1.6217067007 | 0.8084183415 |
| C5 | 1.6214558700 | 1.9916992865 | 2.1448232307 |
| C6 | 0.5644671878 | 2.6757449904 | 2.7364584262 |
| C7 | -0.5663222460 | 2.9671930311 | 1.9814545803 |

| | | | |
|---|---|---|---|
| C8 | -0.6136599914 | 2.5649505336 | 0.6436590491 |
| C9 | -1.7692267854 | 2.8237634487 | -0.2526699631 |
| C10 | -2.9185824610 | 3.4944642969 | 0.1720570645 |
| C11 | -3.9655083962 | 3.7067630420 | -0.7146636535 |
| C12 | -3.8439447871 | 3.2415610052 | -2.0195486308 |
| C13 | -2.6789797358 | 2.5816539068 | -2.3846568718 |
| H14 | 2.2879810563 | 1.0867348346 | 0.2779631742 |
| H15 | 2.5176308443 | 1.7472549913 | 2.7005308694 |
| H16 | 0.6159989245 | 2.9811668099 | 3.7749468713 |
| H17 | -1.3913186814 | 3.4988294014 | 2.4348696249 |
| H18 | -2.9974311916 | 3.8496524078 | 1.1898243765 |
| H19 | -4.8590660564 | 4.2263279298 | -0.3903428892 |
| H20 | -4.6315051084 | 3.3822987905 | -2.7483384731 |
| H21 | -2.5343126207 | 2.2007972341 | -3.3852165333 |
| Cl22 | 2.1205253302 | 0.2994752833 | -2.4493901154 |
| H23 | -0.2451527605 | 1.0844116071 | -3.5001645612 |

2- bipyr-Cl-LACV3P**++
Gas phase Energy: -1233.52534874932 hartrees
Zero Point Energy: 108.211 kcal/mol
Free Energy: -30.587 kcal/mol
final geometry:

| | angstroms | | |
|---|---|---|---|
| atom | x | y | z |
| Pd1 | 0.4982318201 | 0.1413826052 | -0.1811112249 |
| N2 | 0.2374202279 | 0.1255041517 | 1.8894599032 |
| N3 | 2.5681886661 | 0.0213714097 | 0.5766150558 |
| C4 | -0.9600392682 | 0.1788183515 | 2.4970055349 |
| C5 | -1.1029132779 | 0.1700095867 | 3.8775320732 |
| C6 | 0.0405185910 | 0.1033368254 | 4.6663020125 |
| C7 | 1.2804832973 | 0.0469208884 | 4.0442468816 |
| C8 | 1.3625285860 | 0.0583538849 | 2.6499633583 |
| C9 | 2.6552217881 | -0.0018440233 | 1.9215922244 |
| C10 | 3.8982785047 | -0.0795816734 | 2.5560934733 |
| C11 | 5.0516195241 | -0.1331865171 | 1.7810577049 |
| C12 | 4.9427531835 | -0.1080768148 | 0.3942372482 |
| C13 | 3.6734112863 | -0.0296842587 | -0.1701454740 |
| H14 | -1.8165951500 | 0.2279674697 | 1.8404697192 |
| H15 | -2.0923944008 | 0.2144883282 | 4.3136140154 |
| H16 | -0.0290247604 | 0.0947592535 | 5.7474043118 |
| H17 | 2.1793761914 | -0.0058911757 | 4.6424760751 |
| H18 | 3.9749322900 | -0.0991096592 | 3.6345831690 |
| H19 | 6.0227135728 | -0.1940267930 | 2.2584179403 |
| H20 | 5.8176194032 | -0.1481849042 | -0.2419221177 |
| H21 | 3.5075992768 | -0.0056906974 | -1.2423888182 |
| H22 | -0.9825373907 | 0.2244279730 | -0.5681913411 |

| | | | |
|---|---|---|---|
| O23 | -4.3594164839 | -0.4411991776 | -0.5254864770 |
| O24 | -4.1853324627 | -0.0745631971 | 0.6094559200 |
| Cl25 | 0.9451539181 | 0.1505322409 | -2.4615852449 |

3A- bipyr-Cl-LACV3P**++
Gas phase Energy: -1233.53997117057 hartrees
Zero Point Energy: 110.195 kcal/mol
Free Energy: -27.819 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | -0.0771774637 | 1.1273795139 | -1.9023488643 |
| N2 | 0.1614194582 | 1.8758983779 | 0.1937200937 |
| N3 | -1.7302648828 | 2.5798332904 | -1.5813907280 |
| C4 | 1.1256672353 | 1.4729206182 | 1.0284651567 |
| C5 | 1.2367799165 | 1.9456836776 | 2.3311197352 |
| C6 | 0.3026477685 | 2.8746516117 | 2.7774954079 |
| C7 | -0.7000445806 | 3.2942126317 | 1.9118263566 |
| C8 | -0.7506279124 | 2.7774232811 | 0.6133388831 |
| C9 | -1.7926232455 | 3.1766145954 | -0.3749335835 |
| C10 | -2.7904957798 | 4.1147831990 | -0.0952296336 |
| C11 | -3.7250577688 | 4.4279987121 | -1.0757475965 |
| C12 | -3.6466290436 | 3.8012317396 | -2.3149299830 |
| C13 | -2.6271125891 | 2.8791931400 | -2.5260168882 |
| H14 | 1.8246291660 | 0.7478114419 | 0.6273528846 |
| H15 | 2.0344792976 | 1.5912716240 | 2.9713449018 |
| H16 | 0.3510205150 | 3.2686867270 | 3.7858471944 |
| H17 | -1.4319931585 | 4.0144496393 | 2.2501066108 |
| H18 | -2.8441236149 | 4.5994562511 | 0.8697984317 |
| H19 | -4.5034656126 | 5.1536827800 | -0.8712115663 |
| H20 | -4.3544825166 | 4.0166369285 | -3.1050206978 |
| H21 | -2.5048471870 | 2.3544902002 | -3.4674157295 |
| H22 | 1.1389090927 | -0.6323111209 | -3.6390661875 |
| O23 | 1.6371538824 | -0.2393724864 | -1.8907236915 |
| O24 | 1.8693016321 | -0.9353722656 | -3.0055902525 |
| Cl25 | -0.4751406905 | 0.3916607351 | -4.2566559712 |

4- bipyr-Cl-LACV3P**++
Gas phase Energy: -1233.56976597785 hartrees
Zero Point Energy: 111.672 kcal/mol
Free Energy: -26.165 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | -0.0064678342 | 1.2684574321 | -1.9574628031 |
| N2 | 0.2234414940 | 1.8308804159 | 0.0216860748 |

| | | | |
|---|---|---|---|
| N3 | -1.6537478376 | 2.5524034646 | -1.6974421602 |
| C4 | 1.2150461019 | 1.3843286596 | 0.8003370045 |
| C5 | 1.3260580130 | 1.7753481525 | 2.1293004960 |
| C6 | 0.3770332911 | 2.6485337361 | 2.6514662919 |
| C7 | -0.6514446102 | 3.1067600790 | 1.8347103494 |
| C8 | -0.7112916010 | 2.6812979155 | 0.5076338884 |
| C9 | -1.7579680629 | 3.0911457263 | -0.4571481065 |
| C10 | -2.7994014209 | 3.9660651152 | -0.1484301001 |
| C11 | -3.7367479552 | 4.2829881827 | -1.1253222958 |
| C12 | -3.6152074504 | 3.7195140120 | -2.3906753602 |
| C13 | -2.5552464943 | 2.8551483945 | -2.6390371243 |
| H14 | 1.9036344989 | 0.7045421441 | 0.3069875588 |
| H15 | 2.1400739347 | 1.3974203073 | 2.7342272278 |
| H16 | 0.4330298951 | 2.9707827840 | 3.6844237534 |
| H17 | -1.3960064589 | 3.7841370383 | 2.2299238594 |
| H18 | -2.8807408887 | 4.3961203757 | 0.8404335531 |
| H19 | -4.5501402531 | 4.9616234420 | -0.8977614603 |
| H20 | -4.3229824919 | 3.9399972781 | -3.1792329670 |
| H21 | -2.3951912741 | 2.3796880680 | -3.6000652394 |
| H22 | 1.3325216378 | -1.1519229449 | -3.1732597971 |
| O23 | 1.6572655194 | 0.1925827160 | -1.8917471089 |
| O24 | 1.4112657693 | -1.1823070106 | -2.2061109573 |
| Cl25 | -0.3993223486 | 0.7219521346 | -4.2197233188 |

TS1- bipyr-Cl-LACV3P**++
Gas phase Energy: -1233.50271634513 hartrees
Zero Point Energy: 106.013 kcal/mol
Free Energy: -27.982 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1485.82 $cm^{-1}$)
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.3142356383 | 0.0816523560 | -0.1274619006 |
| N2 | 0.1376656915 | 0.0858444164 | 1.9736827958 |
| N3 | 2.4230427801 | 0.0463914936 | 0.5714282298 |
| C4 | -1.0376791750 | 0.1090945084 | 2.6229650290 |
| C5 | -1.1273280774 | 0.1216179447 | 4.0097483840 |
| C6 | 0.0471981984 | 0.1082756828 | 4.7543021189 |
| C7 | 1.2651533240 | 0.0802401240 | 4.0857357909 |
| C8 | 1.2930056514 | 0.0675901798 | 2.6891380842 |
| C9 | 2.5590903566 | 0.0327554625 | 1.9115007049 |
| C10 | 3.8279503298 | -0.0139502231 | 2.4975460097 |
| C11 | 4.9520269320 | -0.0445487550 | 1.6783603986 |
| C12 | 4.7905008341 | -0.0278597753 | 0.2959317194 |
| C13 | 3.4984885490 | 0.0178138756 | -0.2194618303 |
| H14 | -1.9268695703 | 0.1139157389 | 2.0030130876 |

| | | | |
|---|---|---|---|
| H15 | -2.1007539932 | 0.1413129537 | 4.4824716415 |
| H16 | 0.0194511633 | 0.1189679147 | 5.8374167837 |
| H17 | 2.1869524269 | 0.0694472372 | 4.6502124161 |
| H18 | 3.9465361134 | -0.0286322517 | 3.5721577251 |
| H19 | 5.9417552332 | -0.0816909857 | 2.1181383738 |
| H20 | 5.6407445186 | -0.0505054529 | -0.3736480775 |
| H21 | 3.2926680291 | 0.0316634955 | -1.2847053974 |
| H22 | -1.3211417796 | 0.0968461348 | -0.4991581479 |
| O23 | -2.6138843976 | 0.1039889642 | -0.7545023237 |
| O24 | -3.3213138370 | -0.0520019841 | 0.2754583246 |
| Cl25 | 0.6245973558 | 0.0756234583 | -2.4336719061 |

1-bipyr-Cl-BP86
Gas phase Energy: -1083.09743546686 hartrees
Zero Point Energy: 103.246 kcal/mol
Free Energy: -25.564 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.0961309136 | 1.3897375299 | -2.0232306503 |
| N2 | 0.4266034240 | 1.8920002350 | 0.0679362381 |
| N3 | -1.6477761700 | 2.3578985907 | -1.5475907809 |
| C4 | 1.5242773864 | 1.6030893229 | 0.7925432428 |
| C5 | 1.6457332124 | 1.9723649360 | 2.1391008493 |
| C6 | 0.5856192984 | 2.6650318987 | 2.7434020088 |
| C7 | -0.5554465803 | 2.9643572438 | 1.9891732449 |
| C8 | -0.6124221538 | 2.5630445588 | 0.6399617689 |
| C9 | -1.7651979323 | 2.8209257913 | -0.2560607431 |
| C10 | -2.9259416050 | 3.4965573941 | 0.1619730575 |
| C11 | -3.9783109152 | 3.7052712879 | -0.7345930834 |
| C12 | -3.8482788115 | 3.2285920228 | -2.0478222393 |
| C13 | -2.6745775604 | 2.5642613021 | -2.4130959759 |
| H14 | 2.3051221969 | 1.0611170318 | 0.2451122471 |
| H15 | 2.5520776457 | 1.7208572869 | 2.6966800382 |
| H16 | 0.6438941184 | 2.9707442661 | 3.7928381519 |
| H17 | -1.3872895583 | 3.5034719772 | 2.4496734848 |
| H18 | -3.0043776497 | 3.8583610454 | 1.1901399704 |
| H19 | -4.8825475513 | 4.2302968370 | -0.4128990960 |
| H20 | -4.6419710753 | 3.3658449590 | -2.7868677181 |
| H21 | -2.5193805793 | 2.1737633122 | -3.4197476233 |
| Cl22 | 2.1129648632 | 0.3156211732 | -2.4413731217 |
| H23 | -0.2481417358 | 1.0894399555 | -3.4942071749 |

2- bipyr-Cl-BP86
Gas phase Energy: -1233.42536071306 hartrees
Zero Point Energy: 105.727 kcal/mol

Free Energy: -30.543 kcal/mol

final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.4330841170 | 0.1020547653 | -0.1605552695 |
| N2 | 0.1759605705 | 0.1097285477 | 1.8763750101 |
| N3 | 2.4888999434 | 0.0114380520 | 0.5460945492 |
| C4 | -1.0292583949 | 0.1589176801 | 2.4989079233 |
| C5 | -1.1616078155 | 0.1614825966 | 3.8901604237 |
| C6 | -0.0056155914 | 0.1114680517 | 4.6820841900 |
| C7 | 1.2394149746 | 0.0605739128 | 4.0477490741 |
| C8 | 1.3179964174 | 0.0603463180 | 2.6434369066 |
| C9 | 2.6018923073 | 0.0078479976 | 1.9039238967 |
| C10 | 3.8670067998 | -0.0427895392 | 2.5212335717 |
| C11 | 5.0155034021 | -0.0892367550 | 1.7216614844 |
| C12 | 4.8806915491 | -0.0845702398 | 0.3251597868 |
| C13 | 3.5924948003 | -0.0332006032 | -0.2239607649 |
| H14 | -1.8991033246 | 0.1949759592 | 1.8405994546 |
| H15 | -2.1596106683 | 0.2018501702 | 4.3345035377 |
| H16 | -0.0703244304 | 0.1115208049 | 5.7741218277 |
| H17 | 2.1539114258 | 0.0205158336 | 4.6441764069 |
| H18 | 3.9592070753 | -0.0454412401 | 3.6103493326 |
| H19 | 6.0052172193 | -0.1284947081 | 2.1873860317 |
| H20 | 5.7546305754 | -0.1198783542 | -0.3309703377 |
| H21 | 3.3987807736 | -0.0255944513 | -1.3035671198 |
| H22 | -1.0562175663 | 0.1720139161 | -0.5440785941 |
| O23 | -3.4403965586 | -0.2476865646 | -0.4898325803 |
| O24 | -3.9014911100 | 0.0636587779 | 0.6124092890 |
| Cl25 | 0.8431361313 | 0.0906288948 | -2.4476204213 |

3A- bipyr-Cl-BP86

Gas phase Energy: -1233.44267143379 hartrees

Zero Point Energy: 107.511 kcal/mol

Free Energy: -28.009 kcal/mol

final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | -0.0787952731 | 1.1785043712 | -1.8753033150 |
| N2 | 0.2816932954 | 1.9825291370 | 0.0928528313 |
| N3 | -1.8200442734 | 2.3858615473 | -1.5413685694 |
| C4 | 1.2602448737 | 1.5675181084 | 0.9290641750 |
| C5 | 1.2870604902 | 1.9101703562 | 2.2844220827 |
| C6 | 0.2361729977 | 2.6899965948 | 2.8030599345 |
| C7 | -0.7927951759 | 3.0993963151 | 1.9493457111 |
| C8 | -0.7467271078 | 2.7458217170 | 0.5854344109 |
| C9 | -1.7724070028 | 3.1412886487 | -0.3965901780 |

| | | | |
|---|---|---|---|
| C10 | -2.6567317746 | 4.2227444694 | -0.2106047973 |
| C11 | -3.6142376177 | 4.5047907337 | -1.1893076369 |
| C12 | -3.6592554948 | 3.7136842436 | -2.3526197866 |
| C13 | -2.7324252281 | 2.6776310980 | -2.4978859914 |
| H14 | 2.0376981199 | 0.9488578513 | 0.4684567136 |
| H15 | 2.1141610291 | 1.5741765391 | 2.9155788542 |
| H16 | 0.2128776966 | 2.9601407107 | 3.8632388672 |
| H17 | -1.6419873108 | 3.6689084398 | 2.3373177079 |
| H18 | -2.5745571747 | 4.8488967718 | 0.6824229630 |
| H19 | -4.3070271754 | 5.3415051506 | -1.0564337295 |
| H20 | -4.3979831842 | 3.8960634955 | -3.1377090634 |
| H21 | -2.6900174620 | 2.0420182516 | -3.3883833297 |
| H22 | 1.0550029022 | -0.5904762659 | -3.5694545711 |
| O23 | 1.5796636242 | -0.0850088240 | -1.8368056529 |
| O24 | 1.7812949789 | -0.9084020470 | -2.9097826833 |
| Cl25 | -0.4921298592 | 0.4640987246 | -4.2093386664 |

4- bipyr-Cl-BP86
Gas phase Energy: -1233.47563771241 hartrees
Zero Point Energy: 108.949 kcal/mol
Free Energy: -27.613 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.0051919159 | 1.2904426417 | -1.9446640966 |
| N2 | 0.2163814061 | 1.8247083270 | 0.0195439207 |
| N3 | -1.6388046747 | 2.5572494759 | -1.7117808516 |
| C4 | 1.2111628367 | 1.3624469722 | 0.8080585108 |
| C5 | 1.3312712405 | 1.7663057279 | 2.1425073656 |
| C6 | 0.3883139710 | 2.6668225819 | 2.6652160397 |
| C7 | -0.6427268509 | 3.1379551986 | 1.8420201463 |
| C8 | -0.7152803772 | 2.7015433541 | 0.5068668254 |
| C9 | -1.7591934745 | 3.1059518960 | -0.4608615304 |
| C10 | -2.8251665986 | 3.9717388069 | -0.1576626400 |
| C11 | -3.7715683135 | 4.2690787856 | -1.1460570056 |
| C12 | -3.6351356496 | 3.6946692220 | -2.4192911285 |
| C13 | -2.5527908961 | 2.8416400141 | -2.6654965750 |
| H14 | 1.8875023361 | 0.6606799392 | 0.3026962256 |
| H15 | 2.1494422915 | 1.3784535172 | 2.7551155539 |
| H16 | 0.4533514424 | 3.0000230333 | 3.7054610827 |
| H17 | -1.3839706943 | 3.8387335066 | 2.2345087105 |
| H18 | -2.9164662061 | 4.4059181535 | 0.8412421143 |
| H19 | -4.6060639849 | 4.9407026413 | -0.9226279929 |
| H20 | -4.3526218997 | 3.9018404106 | -3.2178031264 |
| H21 | -2.3722488229 | 2.3572662672 | -3.6316581010 |
| H22 | 1.1940011850 | -1.0614294369 | -3.2209465453 |

| | | | |
|---|---|---|---|
| O23 | 1.6433512860 | 0.1854172359 | -1.8825556424 |
| O24 | 1.3130435520 | -1.1672724290 | -2.2455632212 |
| Cl25 | -0.3197924114 | 0.7722955140 | -4.2473725947 |

TS1- bipyr-Cl-BP86
Gas phase Energy: -1233.41458682824 hartrees
Zero Point Energy: 104.015 kcal/mol
Free Energy: -28.318 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-346.10 $cm^{-1}$)
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.3427857596 | 0.0746935373 | -0.1107524060 |
| N2 | 0.1360581207 | 0.0805520847 | 1.9381542495 |
| N3 | 2.4182769457 | 0.0444468478 | 0.5534220616 |
| C4 | -1.0576136011 | 0.0992766834 | 2.5812670825 |
| C5 | -1.1607063883 | 0.1154718334 | 3.9758512324 |
| C6 | 0.0133368194 | 0.1107149103 | 4.7427784840 |
| C7 | 1.2471155356 | 0.0859684114 | 4.0836816188 |
| C8 | 1.2953928447 | 0.0690207428 | 2.6782373438 |
| C9 | 2.5621044493 | 0.0362746528 | 1.9071545124 |
| C10 | 3.8438144309 | -0.0042613974 | 2.4896847686 |
| C11 | 4.9708575342 | -0.0353080192 | 1.6590063803 |
| C12 | 4.8009994401 | -0.0253677024 | 0.2660793239 |
| C13 | 3.4986297734 | 0.0147816836 | -0.2486603985 |
| H14 | -1.9456760805 | 0.0952037157 | 1.9382370376 |
| H15 | -2.1496598133 | 0.1311237925 | 4.4418383053 |
| H16 | -0.0287895716 | 0.1247942770 | 5.8359973535 |
| H17 | 2.1745399089 | 0.0806587730 | 4.6614003571 |
| H18 | 3.9646237332 | -0.0141922556 | 3.5759894362 |
| H19 | 5.9727771671 | -0.0677972510 | 2.0979568571 |
| H20 | 5.6571147621 | -0.0489061180 | -0.4136424049 |
| H21 | 3.2766564574 | 0.0245487166 | -1.3224206114 |
| H22 | -1.2524655685 | 0.1019982458 | -0.4388956266 |
| O23 | -2.6499229749 | 0.1298096263 | -0.7114384928 |
| O24 | -3.3701926495 | -0.0055466297 | 0.3218574820 |
| Cl25 | 0.6216404618 | 0.0639366588 | -2.4186057898 |

1-bipyr-Cl-BLYP
Gas phase Energy: -1082.69436418879 hartrees
Zero Point Energy: 103.004 kcal/mol
Free Energy: -25.632 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.0996034361 | 1.3812432387 | -2.0427113525 |
| N2 | 0.4306434842 | 1.8990537401 | 0.0895261761 |
| N3 | -1.6649151041 | 2.3672927108 | -1.5388474429 |
| C4 | 1.5272449409 | 1.6158611660 | 0.8239538757 |
| C5 | 1.6409374419 | 1.9880629970 | 2.1726683850 |
| C6 | 0.5740368967 | 2.6781700906 | 2.7710392416 |
| C7 | -0.5652705620 | 2.9727144355 | 2.0088589263 |
| C8 | -0.6160870898 | 2.5696433167 | 0.6567774251 |
| C9 | -1.7737638292 | 2.8288051609 | -0.2425790888 |
| C10 | -2.9348952535 | 3.5077004854 | 0.1795066891 |
| C11 | -3.9913582599 | 3.7205144139 | -0.7142785820 |
| C12 | -3.8688755435 | 3.2458701970 | -2.0304453548 |
| C13 | -2.6964789015 | 2.5782276256 | -2.4012139197 |
| H14 | 2.3147769987 | 1.0771469621 | 0.2890886890 |
| H15 | 2.5439582707 | 1.7409919411 | 2.7344061661 |
| H16 | 0.6247747237 | 2.9850184987 | 3.8188015305 |
| H17 | -1.3983866164 | 3.5082191050 | 2.4658533342 |
| H18 | -3.0118791210 | 3.8690865763 | 1.2054276406 |
| H19 | -4.8913403165 | 4.2465723551 | -0.3880317528 |
| H20 | -4.6640427058 | 3.3865230538 | -2.7647449652 |
| H21 | -2.5489310640 | 2.1903044925 | -3.4078588185 |
| Cl22 | 2.1450335778 | 0.2895968089 | -2.4715768638 |
| H23 | -0.2568800031 | 1.0835556881 | -3.5155621815 |

2- bipyr-Cl-BLYP
Gas phase Energy: -1233.00943299283 hartrees
Zero Point Energy: 105.506 kcal/mol
Free Energy: -31.797 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.2306720991 | 0.6004375064 | -0.1904659747 |
| N2 | -0.0083667773 | 0.4225610640 | 1.8810960414 |
| N3 | 2.2488593154 | -0.0497159169 | 0.4805116974 |
| C4 | -1.1832146083 | 0.6320412941 | 2.5311741049 |
| C5 | -1.3298318234 | 0.4378398793 | 3.9096280592 |
| C6 | -0.2210024669 | 0.0043849772 | 4.6532198033 |
| C7 | 0.9931771560 | -0.2134010957 | 3.9900062664 |
| C8 | 1.0897453608 | 0.0015869245 | 2.6004275831 |
| C9 | 2.3472801927 | -0.2147420274 | 1.8331125502 |
| C10 | 3.5789901352 | -0.5621586872 | 2.4281795427 |
| C11 | 4.7073438187 | -0.7435102300 | 1.6160759533 |
| C12 | 4.5881915383 | -0.5742934185 | 0.2272224510 |
| C13 | 3.3355596606 | -0.2239057586 | -0.3007841401 |
| H14 | -2.0127625656 | 0.9585905888 | 1.9058418311 |

| | | | |
|---|---|---|---|
| H15 | -2.2983414381 | 0.6185269430 | 4.3791836873 |
| H16 | -0.2985706745 | -0.1659980111 | 5.7292877444 |
| H17 | 1.8620603443 | -0.5598155996 | 4.5497811859 |
| H18 | 3.6645327698 | -0.6830892437 | 3.5084912315 |
| H19 | 5.6667778857 | -1.0104227279 | 2.0660585303 |
| H20 | 5.4447748133 | -0.7057528007 | -0.4366884430 |
| H21 | 3.1660682521 | -0.0672870781 | -1.3700362824 |
| H22 | -1.1889302326 | 1.1070155033 | -0.5160860992 |
| O23 | -1.1090550979 | -2.0653797214 | 0.1416033461 |
| O24 | -2.1061140142 | -2.0603021014 | 0.8934086361 |
| Cl25 | 0.6526091908 | 0.7996200738 | -2.5011659462 |

3A- bipyr-Cl-BLYP
Gas phase Energy: -1233.02416754387 hartrees
Zero Point Energy: 107.323 kcal/mol
Free Energy: -28.510 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | -0.0396634748 | 1.1620640176 | -1.9111506500 |
| N2 | 0.3052766417 | 2.0195160582 | 0.1218505547 |
| N3 | -1.8006036592 | 2.4583565982 | -1.5472917385 |
| C4 | 1.2830536607 | 1.6205086859 | 0.9697560299 |
| C5 | 1.3013787769 | 1.9762647109 | 2.3255120516 |
| C6 | 0.2457333080 | 2.7577287271 | 2.8293778321 |
| C7 | -0.7773707142 | 3.1601564625 | 1.9611524181 |
| C8 | -0.7226993989 | 2.7912119610 | 0.5996983833 |
| C9 | -1.7538958086 | 3.1943247054 | -0.3914572812 |
| C10 | -2.6426674320 | 4.2713414404 | -0.1852604784 |
| C11 | -3.6022284149 | 4.5705237951 | -1.1612663233 |
| C12 | -3.6475072266 | 3.7989434823 | -2.3362887714 |
| C13 | -2.7190128202 | 2.7610820819 | -2.4962389910 |
| H14 | 2.0655781817 | 1.0010734001 | 0.5246155779 |
| H15 | 2.1214531596 | 1.6459363095 | 2.9658740852 |
| H16 | 0.2132778668 | 3.0394588940 | 3.8846011250 |
| H17 | -1.6229373514 | 3.7372558578 | 2.3394267069 |
| H18 | -2.5690466013 | 4.8801775434 | 0.7174970865 |
| H19 | -4.2959879883 | 5.4015927240 | -1.0119483429 |
| H20 | -4.3834179793 | 3.9961782078 | -3.1180825076 |
| H21 | -2.6839151055 | 2.1384059891 | -3.3932804457 |
| H22 | 1.1359967663 | -0.6164367745 | -3.6206632463 |
| O23 | 1.6725370492 | -0.0661323208 | -1.8935723628 |
| O24 | 1.8955699996 | -0.8845934129 | -2.9882189103 |
| Cl25 | -0.5434502320 | 0.3653512617 | -4.2540487992 |

4- bipyr-Cl-BLYP

Gas phase Energy: -1233.05549589708 hartrees
Zero Point Energy: 107.323 kcal/mol
Free Energy: -27.713 kcal/mol
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.0090451352 | 1.2658239052 | -1.9544223663 |
| N2 | 0.2206854517 | 1.8214022807 | 0.0380080278 |
| N3 | -1.6623882734 | 2.5524079424 | -1.7004528040 |
| C4 | 1.2188457166 | 1.3671505034 | 0.8314223634 |
| C5 | 1.3286473001 | 1.7663559041 | 2.1697289782 |
| C6 | 0.3726012873 | 2.6541240594 | 2.6934697662 |
| C7 | -0.6613862522 | 3.1179700718 | 1.8669363852 |
| C8 | -0.7248949912 | 2.6880964604 | 0.5263792036 |
| C9 | -1.7741478575 | 3.0957552451 | -0.4430123665 |
| C10 | -2.8367202473 | 3.9674825705 | -0.1337275739 |
| C11 | -3.7859932058 | 4.2776998806 | -1.1177056859 |
| C12 | -3.6572656943 | 3.7109480530 | -2.3963908130 |
| C13 | -2.5793671650 | 2.8511271474 | -2.6506536497 |
| H14 | 1.9072945218 | 0.6767023275 | 0.3339807013 |
| H15 | 2.1471057728 | 1.3850997714 | 2.7832909048 |
| H16 | 0.4289998216 | 2.9818771064 | 3.7341300040 |
| H17 | -1.4101627816 | 3.8056980315 | 2.2619068869 |
| H18 | -2.9232326848 | 4.3980041175 | 0.8648633894 |
| H19 | -4.6134402322 | 4.9525683578 | -0.8864005741 |
| H20 | -4.3747257124 | 3.9277467376 | -3.1899463004 |
| H21 | -2.4103826862 | 2.3749049643 | -3.6195003455 |
| H22 | 1.2435963237 | -1.1557136497 | -3.1856834366 |
| O23 | 1.6727046022 | 0.1668869123 | -1.8950430055 |
| O24 | 1.3414262691 | -1.2165272224 | -2.2044044829 |
| Cl25 | -0.3536588295 | 0.7282714139 | -4.2831290029 |

TS1- bipyr-Cl-BLYP
Gas phase Energy: -1232.99358052127 hartrees
Zero Point Energy: 103.155 kcal/mol
Free Energy: -30.115 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1048.73 $cm^{-1}$)
final geometry:

angstroms

| atom | x | y | z |
|---|---|---|---|
| Pd1 | 0.3126123047 | 0.0678368539 | -0.1330209701 |
| N2 | 0.1411834228 | 0.0774013469 | 1.9680567626 |
| N3 | 2.4467422651 | 0.0361674244 | 0.5671650756 |
| C4 | -1.0482678289 | 0.1040978604 | 2.6242441084 |
| C5 | -1.1394525485 | 0.1199490935 | 4.0221320724 |
| C6 | 0.0427592961 | 0.1084160820 | 4.7787981407 |

| | | | |
|---|---|---|---|
| C7 | 1.2719189103 | 0.0801594271 | 4.1081209970 |
| C8 | 1.3098204602 | 0.0640352534 | 2.6991570902 |
| C9 | 2.5810265003 | 0.0336832836 | 1.9248521079 |
| C10 | 3.8623679000 | 0.0039917828 | 2.5177878733 |
| C11 | 4.9990487798 | -0.0211841912 | 1.6977800022 |
| C12 | 4.8404007405 | -0.0165897269 | 0.3020660527 |
| C13 | 3.5395036689 | 0.0121019053 | -0.2245097232 |
| H14 | -1.9407607550 | 0.1130483040 | 1.9913481288 |
| H15 | -2.1219863034 | 0.1417161656 | 4.4969597340 |
| H16 | 0.0119492470 | 0.1214876006 | 5.8707395968 |
| H17 | 2.2002004827 | 0.0720809731 | 4.6799837322 |
| H18 | 3.9768303764 | -0.0006216294 | 3.6025355296 |
| H19 | 5.9954469909 | -0.0443878044 | 2.1460212169 |
| H20 | 5.7016874641 | -0.0354549899 | -0.3686023441 |
| H21 | 3.3377373954 | 0.0165570154 | -1.2988951634 |
| H22 | -1.3946040450 | 0.0999143979 | -0.4783481321 |
| O23 | -2.6154159053 | 0.1292922636 | -0.7511947653 |
| O24 | -3.3508073321 | 0.0345719507 | 0.3144244432 |
| Cl25 | 0.5648460690 | 0.0587476620 | -2.4789068653 |